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Soberania Nacional

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15 a 18 de junho de 2026
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SOCIEDADE BRASILEIRA DE QUÍMICA

Anais da 49ª Reunião Anual da SBQ

Campinas-SP
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EDITORIAL

Após o sucesso da 48ª RASBQ e diante dos inúmeros pedidos de “bis”, a 49ª Reunião Anual da Sociedade Brasileira de Química retorna a Campinas. Como Secretária-Geral da SBQ e presidente da comissão organizadora, tenho plena convicção de que esta edição será ainda mais marcante. Há quase cinco décadas, a SBQ promove anualmente este encontro fundamental, reunindo cerca de 2000 participantes e impulsionando avanços em ciência, inovação, educação, políticas públicas, formação de profissionais e disseminação científica. É um espaço de encontros e reencontros que fortalece nossa comunidade e reafirma o pertencimento à SBQ (#ASBQéNossa). Trata-se de um dos maiores eventos de Química da América Latina e um dos mais relevantes do Brasil, palco de oportunidades e inspiração para gerações de estudantes, cientistas, professores e profissionais.

O tema da 49ª RASBQ de 2026 — “Química para a Soberania Nacional” — é urgente e estratégico. Em um cenário internacional marcado por disputas tecnológicas e pela valorização de recursos naturais, discutir soberania significa defender o direito do Brasil de decidir sobre suas riquezas, seu beneficiamento e sua aplicação em benefício da sociedade. A Química é central nesse processo: está presente em tecnologias de ponta, na saúde, na energia, na agricultura, em fontes renováveis, na sustentabilidade e na resposta às emergências climáticas. Um país soberano precisa dominar o conhecimento científico e tecnológico que sustenta sua independência. No Brasil, a Química se destaca pela abundância de recursos naturais, pela excelência em pesquisa e inovação e pela força de sua indústria. Soberania nacional também é soberania científica. Sem ciência forte e independente, não há soberania plena.

Durante quatro dias intensos, a 49ª RASBQ oferecerá uma programação rica, com mais de 100 palestrantes e 1120 trabalhos apresentados em 3 sessões de painéis. Temos participantes inscritos de 15 países diferentes e de praticamente todos os estados brasileiros (26 das 27 unidades federativas). Nas sessões coordenadas, teremos cerca de 140 apresentações orais distribuídas entre docentes, pesquisadores, pós-doc e estudantes de pós-graduação. Nas sessões de flash presentations, teremos 32 apresentações orais de estudantes de iniciação científica. Como tradição, teremos a SBQ na Escola, um espaço para promover divulgação científica entre alunos de escola pública e que recebe cerca de 500 estudantes do ensino médio todo ano. Teremos novidades quanto às visitas do CNPEM – serão ampliadas além do SIRIUS. Inclusão e acessibilidade seguem como compromissos centrais: desde a ficha de inscrição, definição da programação até a infraestrutura do evento, com espaços família, sala quieta para pessoas neurodivergentes e opções de espaço kids. Campinas, polo científico e tecnológico, acolhe novamente a SBQ em um ambiente totalmente acessível.

A SBQ, idealizadora desse evento, é uma das mais importantes sociedades científicas brasileiras, com grande inserção na comunidade internacional e está prestes a festejar suas bodas de ouro com a comunidade, em 2027. Ela é formada por uma grande equipe que trabalha voluntariamente pela sociedade: diretoria e conselho consultivo, conselho fiscal, 13 divisões científicas, 26 secretarias regionais, comitê Jovens Pesquisadores, Núcleo Mulheres e Núcleo de Inclusão e Diversidade. Conta ainda com uma equipe incrível de secretaria (Rosângela, Cleuza e Telma), sistema (APTOR, especialmente Leandro), assessoria de imprensa (Mario), gerente de evento (Alexandre) e comunicação (Instituto Sua Ciência, especialmente Juliana e Jéssica), que trabalham arduamente pela SBQ. O sucesso da 49ª RASBQ se deve a toda essa equipe.

Agradecemos também a todos os apoiadores, patrocinadores e expositores do evento. Em especial, destacamos o apoio do CNPEM, ABIQUIM, PROFQUI, ACS, RSC e CFQ.

Para finalizar, o ano de 2026 será decisivo para o Brasil com as eleições nacionais. Nesse contexto, o tema da nossa reunião ganha ainda mais relevância: defender a soberania nacional é responsabilidade de todos nós. A Química, como ciência estratégica, nos dá instrumentos para transformar recursos em desenvolvimento, conhecimento em independência e inovação em futuro. Que a 49ª RASBQ seja palco de debates profundos e nos inspire a fortalecer a soberania científica e tecnológica do Brasil, condição essencial para uma soberania nacional plena. A SBQ é Nossa e o Brasil também é.

Elisa S. Orth
Secretária Geral da SBQ (2024-2026)
Presidenta da Comissão Organizadora da 49ª RASBQ

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49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

AMB - Química Ambiental

Acceleration of Oil–Water Separation in Produced Water by Low-Concentration ZIF-8 Suspensions

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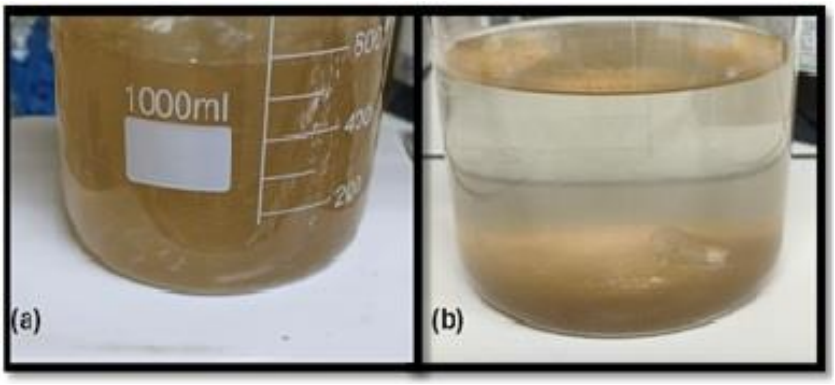
Palavras Chave:*Produced water; Oil–water separation; ZIF-8; MOF*

Highlights

Suspended ZIF-8 destabilized oil-in-water emulsions.
Treated water showed a visual clarification, indicating emulsion breakdown.
ZIF-8 shows strong potential for produced water treatment in oil fields.

Resumo/Abstract

Produced water (PW) from oil and gas extraction typically contains highly stable oil-in-water (O/W) emulsions, which hinder conventional gravitational separation and necessitate alternative physicochemical approaches, particularly in mature oilfields with high oil-to-water ratios. This study evaluated the effectiveness of suspended ZIF-8 (zeolite imidazolate framework-8) as a destabilizing agent for synthetic PW emulsions, with emphasis on phase segregation behavior and visual separation efficiency. A volume of 0.6 L of synthetic PW was prepared as O/W emulsion, and all experiments were conducted at 25 °C under atmospheric pressure. A low-concentration ZIF-8 suspension (0.5 g L^{-1}) was directly added to the emulsion, followed by mechanical stirring at 200 rpm for 15 min. A control system without ZIF-8 addition was also evaluated and exhibited high emulsion stability, with negligible gravitational separation even after 72 h of static sedimentation. In contrast, the ZIF-8-treated systems showed a marked enhancement in phase separation. After 24 h of rest, a significant fraction of the oily phase co-settled with the ZIF-8 suspension, indicating effective destabilization of the dispersed droplets. In addition, a residual oil layer accumulated at the surface and could be readily removed, highlighting the practical applicability of this approach for field-scale operations. Visual changes in the treated water were also observed, including a reduction in color intensity, residual turbidity, and a transition from diffuse light scattering to a milky translucent appearance, attributed to suspended ZIF-8 particles (Fig.1). Overall, the results demonstrate that the ZIF-8 exhibits potential to accelerate emulsion breakdown and gravitational segregation in PW systems. This strategy is particularly relevant for oilfields affected by stable emulsions, offering prospects for reduced residence times, improved operational efficiency, and enhanced water management.



(a) Untreated stable O/W emulsion; (b) treated sample with ZIF-8, exhibiting phase segregation.

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Activated carbon from banana pseudostem for caffeine removal

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Palavras Chave:*adsorption,emerging contaminants,kinetic,microporous,residue*

Highlights

Adsorption equilibrium in around 30 min;
Approximately 20 mg·L^{-1} of caffeine was removed after 120 min of adsorption;
Hydrothermal treatment and $ZnCl_2$ activation improved the caffeine adsorption.

Resumo/Abstract

Caffeine is partly removed during wastewater treatment and frequently detected in water bodies. In Brazil, it is not legally monitored and may occur at 47.5–753.5 µg·L^{-1}.[1,2] The Maciço de Baturité region (CE) is an important banana-producing area, yet about 60% of the biomass is discarded.[3] This study proposed producing activated carbon from this residue, chemically modified with $ZnCl_2$, and evaluating its efficiency for caffeine removal. The synthesis involved hydrothermal treatment,[4] impregnation with $ZnCl_2$ (1:1-1:3 %w/w) and pyrolysis (600 °C/1 h), yielding CZ1, CZ2, and CZ3. A control activated carbon (CC) was prepared only by pyrolysis. All adsorbents were characterized by XRD and FTIR. The adsorption tests were carried out using a 20 mg·L^{-1} caffeine solution, according to the literature,[5] under agitation at 200 rpm for up to 120 min. The adsorption capacity (q_e) was determined by UV–Vis at 273 nm and the experiments were performed in triplicate. XRD showed that $ZnCl_2$ activation promoted an amorphous carbon structure, while CC exhibited residual non-carbonized biomass. FTIR confirmed typical functional groups and inorganic content. The RB showed no adsorption; the hydrothermally treated material (RB-H) achieved 8.0 mg·g^{-1} and CC reached 5.0 mg·g^{-1} after 120 min. In contrast, CZ1, CZ2, and CZ3 achieved 19.7, 19.8, and 20 mg·g^{-1}, respectively, reaching equilibrium*ca.* 30 min. The efficiency is attributed to $ZnCl_2$ acting as a dehydrating agent, generating a predominantly microporous structure.[4] Banana residue is a promising precursor for activated carbon capable of completely removing caffeine at 20 mg·L^{-1}.

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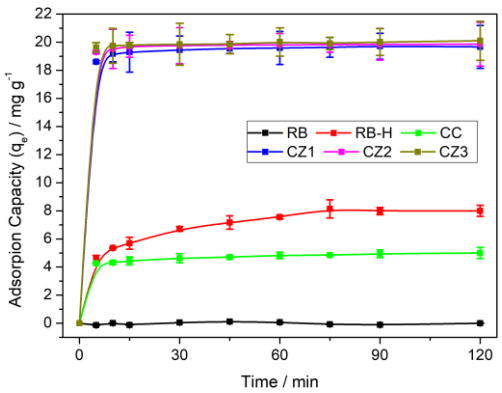


Figure 1. Caffeine adsorption kinetic on different synthesized adsorbents.

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ADSORÇÃO DE PARACETAMOL EM MEIO AQUOSO UTILIZANDO RESÍDUOS DE SACHA INCHI

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Palavras Chave:*Adsorção,Fármacos,Biomassa,Recursos hídricos,Biocarvão*

Highlights

Sustainable materials from residual biomass applied to drug removal. Efficient adsorption of paracetamol, ibuprofen, tetracycline and ketoprofen.Eco-friendly solution for water treatment.

Resumo/Abstract

A contaminação de recursos hídricos por fármacos tem aumentado significativamente devido ao elevado consumo e ao descarte inadequado desses compostos. Os sistemas convencionais de tratamento de esgoto não foram projetados para remover micropoluentes emergentes, o que reduz sua eficiência na eliminação dessas substâncias. Nesse contexto, tecnologias complementares, como o processo de adsorção, vêm sendo investigadas como alternativas promissoras para o tratamento de águas contaminadas. Neste estudo avaliou-se o potencial de resíduos de biomassa lignocelulósica como adsorventes sustentáveis para a remoção de paracetamol em meio aquoso. Foi utilizado o resíduo de sacha inchi (Plukenetia volubilis), planta perene da família Euphorbiaceae encontrada na região amazônica. Seus frutos apresentam formato estrelado e contêm cápsulas onde se localizam as sementes. A casca proveniente do processo de extração de óleo foi triturada e peneirada em malha de 32 mesh (500 µm) e posteriormente seca em estufa a 105 °C por 24 h. A caracterização morfológica foi realizada por microscopia eletrônica de varredura (MEV) e a composição elementar semiquantitativa por EDX. Os grupos funcionais foram identificados por espectroscopia no infravermelho com transformada de Fourier (FTIR) na faixa de 4000–400 cm^{-1}.Os ensaios de adsorção foram realizados em reator de leito fixo à temperatura ambiente, utilizando biomassa in natura e biochar obtido por pirólise a 450 °C por 180 min. A concentração de paracetamol foi determinada por CG/MS. O FTIR da sacha inchi calcinada apresentou bandas de carbonatos (1300–960 e 800–690 cm^{-1}), enquanto a biomassa in natura mostrou bandas típicas de celulose: O–H (~3317 cm^{-1}), C–H (~2920 cm^{-1}) e C–O–C. Os resultados iniciais foram promissores apresentando uma redução de 43% na concentração de paracetamol, ao utilizar este resíduo de biomassa como adsorvente sustentável.

Adsorption of 4-tert-Octylphenol onto PET and PE: The Role of Microplastic Concentration and Aging

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Palavras Chave:*Adsorption,Microplastics,4-Tertocylphenol,Polyethylene Terephthalate (PET),Polyethylene (PE)*

Highlights

4-tOP adsorption was evaluated on virgin and aged PET and PE.

Removal increased with MP concentration.

PE reached 92.8% removal and PET 61.2% at 5 g L^{-1}.

Aging reduced removal on PET.

Resumo/Abstract

The accumulation of microplastics (MPs) in aquatic systems has raised concerns regarding their role as carriers of hydrophobic organic contaminants. Among these compounds, 4-tert-octylphenol (4-tOP) is frequently detected due to its endocrine-disrupting properties and environmental persistence.[1,2] This study evaluates how polymer type, artificial aging (virgin and artificially aged), and microplastic concentration influence 4-tOP adsorption onto PET and PE microplastics (0.15–0.42 mm). Virgin and artificially aged polyethylene terephthalate (PET) and polyethylene (PE) were compared. Aging was induced by UVC irradiation (15W, 254 nm) for 96 h, and surface modifications were monitored by FTIR spectroscopy. Batch experiments were conducted using 40 mL of 4-tOP solution (5 mg L^{-1}) at 25 °C for 24 h under agitation (150 rpm), varying microplastic concentration from 0.25 to 5.0 g L^{-1}. After contact, suspensions were centrifuged and residual 4-tOP concentrations in the supernatant were determined by UV–Vis spectroscopy. All adsorption experiments were performed in duplicate. The highest removal efficiencies were observed at 5.0 g L^{-1} for both polymers under virgin and aged conditions. Under this condition, PE achieved 92.3% (virgin) and 92.8% (aged) removal. For PET, removal reached 61.2% (virgin) and decreased to 53.3% after aging. Overall removal ranged from 53.3% to 92.8%, depending on polymer type and aging condition. These results demonstrate that polymer type and microplastic concentration govern 4-tOP removal efficiency, with polymer-dependent aging effects. Such differences may influence the environmental sorption behavior of hydrophobic contaminants in aquatic systems.

[1] Journal of Hazardous Materials 495 (2025) 138934

[2] Environmental Pollution 340 (2024) 122754

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Adsorption of amoxicillin and methylene blue from aqueous media using commercial activated carbon

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Palavras Chave:*Activated carbon, adsorption, emerging contaminants, dyes, green chemistry,Activated carbon,adsorption,emerging contaminants,dyes,green chemistry*

Highlights

Activated carbon shows high adsorption of contaminants.

It efficiently removes pharmaceuticals and dyes.

Rapid initial adsorption of methylene blue was observed.

Resumo/Abstract

Water pollution is a global environmental and public health issue associated with the improper disposal of waste, including pharmaceuticals and other organic contaminants. In this context, carbon-based materials have been investigated as sustainable and low-cost alternatives for the removal of emerging contaminants from water. This study evaluated a commercial activated carbon (CAC) from ISOFAR (Rio de Janeiro, Brazil) for the adsorption of amoxicillin and methylene blue in aqueous medium. The adsorbent presented a specific surface area of 745 $m^2\ g^{-1}$ and a point of zero charge (pHPZC) of 3.14. Quantification was performed by UV-Vis spectrophotometry at 230 nm (amoxicillin) and 662 nm (methylene blue), following ANVISA Resolution No. 166/2017. Adsorption kinetics were conducted using 10 mg of activated carbon and 10 mL of contaminant solution (100 mg L^{-1}) at 25 °C. Methylene blue reached equilibrium within 5 min, with an adsorption capacity of 66.6 mg g^{-1}, while amoxicillin reached equilibrium at 60 min, with a capacity of 45.6 mg g^{-1}. The lower adsorption of amoxicillin is attributed to electrostatic repulsion at neutral pH. The results demonstrate the efficiency of commercial activated carbon for removing emerging contaminants.

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Agradecimentos/Acknowledgments

FAPERJ

ADSORPTION OF BORDEAUX RED FOOD DYE ONTO ACTIVATED CARBON: KINETIC AND EQUILIBRIUM STUDIES

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Palavras Chave:*Keywords: carbon materials; environmental remediation; organic pollutants.*

Highlights

The Elovich model best described the kinetic data.

The Freundlich model fitted the equilibrium data well.

The AC is a promising material for the removal of VB from aqueous solution.

Resumo/Abstract

Due to population growth, there has been an exponential increase in the use of food dyes, such as Bordeaux Red (BV), which has potential toxicity, including mutagenic and carcinogenic effects, in addition to posing risks to aquatic life and human health. In this context, the development of effective water treatment methods become crucial. Adsorption processes represent a viable solution, particularly activated carbons(ACs), which can be produced from renewable sources and exhibit a high surface area. This study proposes to investigate the kinetics and equilibrium of BV adsorption on AC produced from castor bean husks and activated with H_3PO_4.

The kinetic profiles presented in Fig. 1a show that VB adsorption exhibits a high initial rate, followed by a slower stage, with a gradual increase in adsorption until equilibrium is reached at 60, 160, and 200 min for solutions with concentrations of 30, 75, and 135 mg L^{-1}, respectively. As time progresses, the adsorption rate decreases due to the saturation of the AC adsorption sites. The pseudo-first-order(PPO), pseudo-second-order (PSO), and Elovich kinetic models were fitted to the experimental data. Among these, the Elovich model provided de best fit, presentingΔq_evalues of 0.18, 2.93, and 2.55% for the studied concentrations, respectively.

Fig. 1b demonstrates that VB adsorption onto AC increases with rising temperature. The adsorption isotherms were classified as type L2, indicating a high affinity between the adsorbate and the adsorbent, which favors monolayer formation as a result of surface sites saturation. The Freundlich model provided the best fit to the experimental data at temperatures of 20, 30, 40, and 50 °C, withΔq_evalues of 0.06, 1.88, 2.85, and 1.08%, respectively, suggesting the occurrence of multilayer adsorption and the coexistence of chemisorption and physisorption mechanisms. Therefore, the studied system can be efficiently applied for the removal of VB dye from aqueous medium.

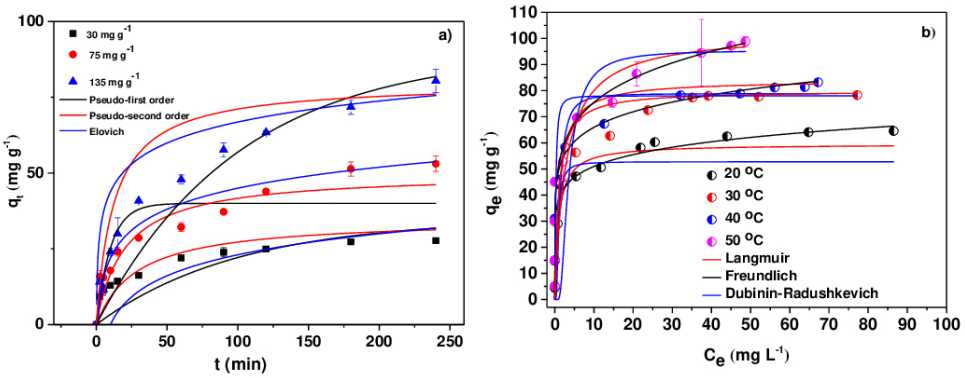


Fig 1. Experimental data and nonlinear model fits for kinetics (a) and equilibrium isotherms (b).

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The researchers express their gratitude for the financial support from CAPES, CNPq, and Fundação Araucária. They also thank UEM-COMCAP and DQI for the physical space and infrastructure.

A fast ultrasound-assisted extraction for As, Cd and Pb determinations in seagrass samples by ICP OES

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Palavras Chave:*seagrass, biomonitoring, Todos os Santos Bay, Ultrasound-assisted extraction.*

Highlights

A green UAE method using diluted HNO_3 was developed for As, Cd, and Pb determination in seagrasses
Factorial design optimization enabled efficient extraction under mild conditions

Resumo/Abstract

The contamination of coastal ecosystems results primarily from anthropogenic activities. Seagrasses stand out as important bioindicators due to their capacity for bioaccumulation and ubiquity. Ultrasound-assisted extraction (UAE) offers low cost, reduced time, moderate temperatures, and the possibility of using diluted acids. His study aimed to develop an UAE procedure using diluted nitric acid for the subsequent determination of arsenic, cadmium, and lead by inductively coupled plasma optical emission spectrometry (ICP OES). A full factorial design with 2 levels (2k) and a central-point replication was employed to evaluate the effects of variables affecting extraction. The variables studied were HNO_3 concentration (1.0–2.0 mol L^{-1}), sonication time (20-40 min), and temperature (40–60 ºC). A certified reference material,*Brachiaria brizantha*cv. Marandu (RM-Agro E1001a) was used in this study. The normalized multiple response, based on the analytical signals obtained from the spectrometric measurements, was used as the design response. The conditions chosen for the proposed extraction procedure were: 40 °C, 20 min of sonication, and HNO_3 concentration of 1.0 mol L^{-1}. The method was validated for LOD (0.10-0.13 mg kg^{-1}) and LOQ (0.45-3.65 mg kg^{-1}), precision (%RSD <5.9%), and accuracy (%recovery 80-110%). The proposed method was applied to seagrass samples collected from three beaches of Todos os Santos Bay (BTS), Bahia, Brazil, with As, Cd, and Pb concentrations ranging from 0.61 ± 0.08 to 4.87 ± 0.14, 0.02 ± 0.01 to 0.13 ± 0.01, and 0.13 ± 0.05 to 0.94 ± 0.09 mg kg^{-1}, respectively. It can be inferred that the proposed method is low-cost, requires less diluted nitric acid, and generates less waste, aligning with green chemistry principles.

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Aging-Driven Changes in PET and PE Microplastics: Impacts on Bisphenol AAdsorption Behavior

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Palavras Chave:*Adsorption,Microplastics,Bisphenol A,Polyethylene Terephthalate (PET),Polyethylene (PE)*

Highlights

BPA adsorption was investigated on virgin and aged PET and PE.
Virgin PET reached 8.7% removal and PE 4.6%.
MP aging reduced BPA adsorption on PET.
Adsorption occurred at different MP concentrations.

Resumo/Abstract

The increasing accumulation of microplastics (MPs) in aquatic environments has raised concerns regarding their role as carriers of endocrine-disrupting compounds. Among these contaminants, bisphenol A (BPA) is frequently detected due to its widespread industrial use and persistence. Evaluating how microplastic transformation affects contaminant behavior contributes to environmental risk assessment.[1,2] In this sense, this study aims to comparatively evaluate BPA adsorption onto virgin and UV aged polyethylene terephthalate (PET) and polyethylene (PE) microplastics (0.15–0.42 mm), considering the influence of microplastic concentration. Aging was induced by UVC irradiation (15 W, 254 nm) for 96 h, and surface modifications were monitored by FTIR spectroscopy. Batch adsorption experiments were performed using 40 mL BPA solutions (5 mg L^{-1}) under controlled conditions (24 h, 25 °C, 150 rpm), varying MP concentration from 0.25 to 5.0 g L^{-1}. Residual BPA concentrations were determined by UV–Vis spectroscopy after centrifugation. For virgin microplastics, maximum BPA removal reached 8.7% for PET at 5.0 g L^{-1} and 4.6% for PE at 4.0 g L^{-1}. PET exhibited slightly higher removal efficiency than PE under the evaluated conditions. After artificial aging, the maximum removal for PET decreased to 6.1% at 0.25 g L^{-1}, whereas PE exhibited its highest removal (5.1%) at 0.75 g L^{-1}. For virgin materials, PET presented higher removal percentages than PE, whereas aging reduced the difference between the polymers. The concentration at which maximum removal occurred differed between virgin and aged materials. These results show that polymer type, aging condition, and microplastic concentration affect BPA distribution in aqueous systems. Understanding these factors is relevant for predicting the environmental behavior of BPA in the presence of microplastics in aquatic environments.

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[2] Journal of Hazardous Materials 424 (2022) 127529

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FAPERGS (RITEs - Inova-Vida RS)

Amazonia carbon uptake is collapsing and shifting from a sink to a source

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Palavras Chave:*Amazonia,CO2,carbon,climate change,deforestation*

Highlights

The Amazon rainforest's ability to remove carbon from the atmosphere is rapidly declining as tree mortality rises and the climatic conditions required to sustain a humid tropical forest deteriorate

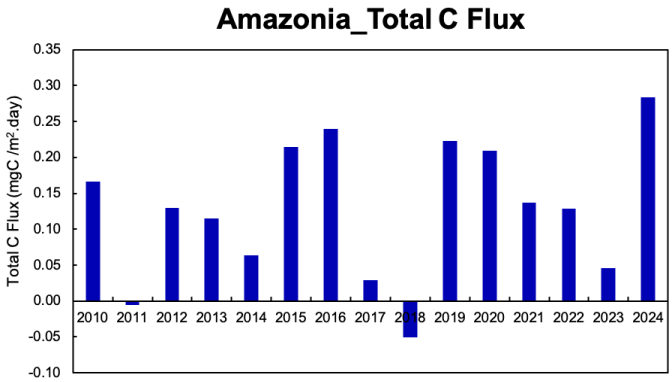
Resumo/Abstract

The Amazon rainforest's ability to remove carbon from the atmosphere is rapidly declining as tree mortality rises and the climatic conditions required to sustain a humid tropical forest deteriorate. Deforestation and degradation are reshaping regional climate—reducing rainfall, raising temperatures, and lengthening the dry season—driving sharp increases in Amazon carbon emissions. Large-scale climate phenomena such as El Niño and warming of the tropical North Atlantic (TNA) further intensify the effects of human activities, including fires, degradation, and forest clearing.

We present a 15-year assessment of the Amazon carbon balance, which averaged 0.32 ± 0.08 PgC yr^{-1}. Fires were the dominant carbon source (0.40 ± 0.07 PgC yr^{-1}), and the forest's carbon uptake has become increasingly insufficient to compensate for these emissions. We used year-to-year variability to examine how carbon emissions relate to human actions, regional climate, and extreme events.

Forest loss reduces precipitation and increases temperature, intensifying climate stress—especially in the most deforested regions—and making the forest increasingly flammable. Although global climate events such as El Niño and TNA warming amplify these regional impacts, they are not the primary cause.

Years with strong carbon uptake were associated with La Niña conditions, while typical years showed a much weaker sink. The highest emissions occurred during periods dominated by deforestation and biomass burning, notably 2019–2022. In 2024, the combination of 60,964 km^2 of deforestation over the previous six years, two strong El Niño and TNA events, and an extensive burned area of 155,413 km^2—23 times larger than the area deforested that year—produced the highest carbon emissions in the 15-year record: 0.75 ± 0.05 PgC yr^{-1}, including 0.80 ± 0.05 PgC yr^{-1} from fires alone.



Annual mean Amazon carbon balance from 2010 to 2024

Agradecimentos/Acknowledgments

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Analysis of sediment from the beaches of Ilhéus - Bahia through the determination of PAHs and Quinones.

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Palavras Chave:*Sediment, Beach, Polycyclic Aromatic Hydrocarbons (PAHs), Quinone, Environmental Contamination.*

Highlights

Simultaneous determine organic compounds (PAHs and quinones) in sediment samples by GC-MS, analyzing the possible origins of these compounds on the beaches of the southern zone of Ilhéus-BA.

Resumo/Abstract

Coastal zones are strategic ecosystems for the economy and ecological balance, making the monitoring of their environmental quality indispensable. This study investigated the occurrence of Polycyclic Aromatic Hydrocarbons (PAHs) and Quinones in surface sediments in the municipality of Ilhéus, Bahia. Due to their carcinogenic potential, persistence, and bioaccumulation, the USEPA classifies 16 PAHs as priority pollutants.ampling was conducted at five distinct points in the Southern Zone of Ilhéus: P1(Near by the airport), P2 (gas station), P3 (residential area), P4 (wholesale district), and P5 (remote zone/Cururupe River). The methodology involved microextraction techniques and analysis by gas chromatography-mass spectrometry (GC-MS). The results confirmed anthropogenic contamination in the region (Figure 01). P2 exhibited the highest pollutant load and compound diversity, characterized by Naphthalene (0.0116 µg/g) and Phenanthrene (0.0394 µg/g). The predominance of low molecular weight PAHs (2-3 rings), such as Naphthalene and Acenaphthylene, suggests a significant contribution from petrogenic sources and the incomplete combustion of fossil fuels associated with intense vehicular traffic and logistical activities near points P2, P3, and P4. Concurrently, the detection of high molecular weight PAHs, such as Dibenzo(a,h)anthracene (0.0142 µg/g) in P4, indicates high-temperature combustion processes (pyrogenic sources). P5 stood out due to the exclusive presence of 9,10-anthraquinone (0.0060 µg/g), an oxygenated derivative pointing to environmental oxidation processes or specific diesel combustion emissions. It is concluded that the environmental quality of Ilhéus' beaches is compromised by distinct anthropogenic inputs, requiring urgent monitoring strategies and coastal management to mitigate risks to the biota and public health.

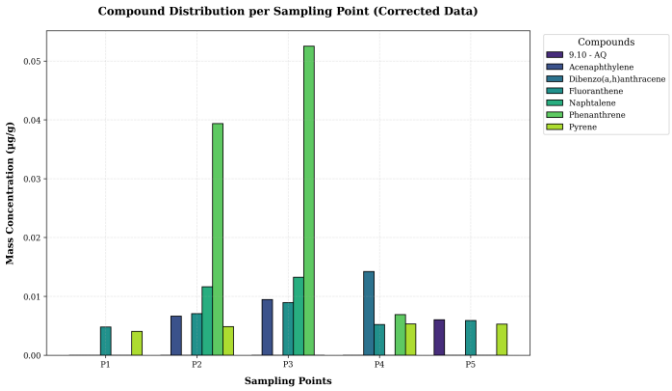


Figure 01: Incidence of PAHs and quinones in sampling locations.

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Southern of Bahia Federal University (UFSB), Federal University of Bahia (UFBA), Science and Energy Interdisciplinar Center (CIENAM), Science and Technology Nacional Institute (INCT).

Application of biochar/ZnCo hydroxyl salt composite in the removal of Diclofenac from aqueous medium by hydrogen peroxide activation

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Palavras Chave:*Biochar,ZnCo hydroxyl salt,composite,Dilofenac degradation,Hydrogen peroxide activation*

Highlights

Successful synthetic of ZnCo double hydroxyl salt composite with BC; Diclofenac removal yielded over 70%; Cobalt cations could be associated to catalytic activity; Radicals were identified in quenchin

Resumo/Abstract

The contamination of aquatic environments by pharmaceuticals is a direct consequence of scientific and technological advances [1]. The widespread use of non-steroidal anti-inflammatory drugs leads to their presence, and that of their metabolites, in water bodies, causing various eco-toxicological effects [2]. In this context, developing new water remediation methods is imperative.In this context, developing efficient remediation methods is imperative. In this work we report the synthesis of peanut-shell biochar (BC) composites with Zn/Co hydroxy salts (ZnCoHS) via controlled precipitation of the inorganic matrix onto the biochar surface.The materials were characterized and applied in the Diclofenac removal from aqueous media, in a reaction with hydrogen peroxide. XRD patterns confirmed the success of the synthesis, with crystalographic peaks matching ZnCoHS sctructure, indicating no phase alteration after anchoring on the biochar.
The removal experiments were performed with synthesized materials (varying BC and ZnCoHS proportion) and with the inorganic matrix (ZnCoHS) and with biochar (BC). Also, a negative control expriment was developed (DCL solution + hydrogen peroxide). The first 30 minutes considered adsorption-dessorption phenomena between DCL and the materials (named t_{-30}); 100 µL of H_2O_2 (30% w/w) was added in the system at t_0 and samples were taken at t_{15}, t_{30}, $t_{45}$and t_{60} (troughout one-hour experiments). The collected samples were analysed in HPLC-DAD.The removal experiments showed improved performance for the composite $BC_{0.75}$@$ZnCoHS_{0.25}$ (75:25 wt), represented in Figure 1. Quenching experiments revealed that superoxide (O_2•$^-$) and hydroxyl (•OH) radicals are the primary active species, with cobalt cations playing a leading role in the catalytic activation.
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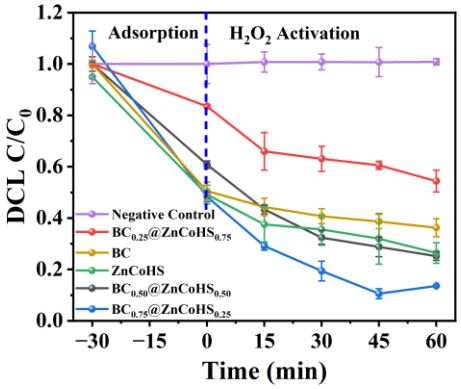


Figure 1 – Diclofenac removal experiments with synthesized materials.

Agradecimentos/Acknowledgments

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Assessment of chemical composition and enrichment factors in settleable dust from Volta Redonda, Rio de Janeiro

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Palavras Chave:*Settleable dust,ICP-MS,Sample preparation,Enrichment factor,Atmospheric pollution*

Highlights

Chemical composition of settleable dust was evaluated by ICP-MS after different sample preparation procedures, and enrichment factors indicated potential anthropogenic influence in the study area.

Resumo/Abstract

In recent decades, the Brazilian steel industry has received substantial investments. In the state of Rio de Janeiro, the city of Volta Redonda stands out, where major industrial activities and potential sources of atmospheric pollution are concentrated. Among the pollutants associated with industrialized areas, settleable dust consists of particles that deposit by gravitational action, generally with diameters larger than 10 µm, and may act as an important source of environmental contamination. The present study aimed to evaluate the chemical composition of settleable dust collected in Volta Redonda, as well as to compare different sample preparation methodologies. Settleable dust and soil samples were subjected to three different preparation protocols: aqueous extraction, HNO_3 leaching, and microwave-assisted acid digestion with HNO_3.The resulting extracts were analyzed by inductively coupled plasma mass spectrometry (ICP-MS). The determined concentrations allowed the assessment of the analytical efficiency of the digestion methodologies, the characterization of the composition of settleable dust, and the calculation of the enrichment factor (EF), a parameter frequently employed as an indicator of possible anthropogenic sources of contamination. The results evidenced higher efficiency of the acid methodologies compared with aqueous extraction, with similar percentage analytical recoveries for most of the investigated elements. In terms of composition, Al and Mg showed major concentrations, whereas Mn, Pb, Sr, Zn, and Ti occurred at minor levels. EF values indicated significant enrichment ($5 < EF < 20$) for Cu, Mn, Pb, and Sr, and moderate enrichment ($2 < EF < 5$) for Ba, Be, Cd, Cr, Mg, V, and Zn. Therefore, the results suggest that the composition of settleable dust collected in the study area is potentially influenced by anthropogenic sources when compared with natural background levels.

Agradecimentos/Acknowledgments

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Assessment of metals in a spring used by riverside communities in southwestern Bahia and implications for environmental and human health.

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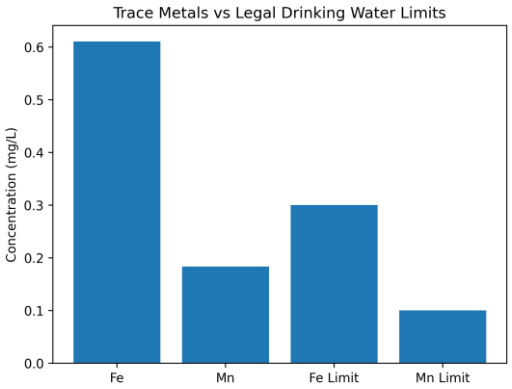
Palavras Chave:*Trace metals,Water quality,Environmental health,Riverside communities,FAAS*

Highlights

Metal contamination detected in a natural spring highlights environmental vulnerability and potential health risks in communities using untreated water sources

Resumo/Abstract

The quality of spring water intended for human supply is a critical public health issue, especially in riverside communities with limited access to centralized treatment systems. This study evaluated the water quality of a spring located in the Mandacaru neighborhood, Jequié, Bahia, Brazil, focusing on metal concentrations and their environmental and sanitary implications. Analyses followed the Standard Methods for the Examination of Water and Wastewater, and metals were determined by Flame Atomic Absorption Spectrometry (FAAS). The investigated elements were Fe, Mn, Ca, Mg, Ni, Cu, Cd, Pb, and Zn. Mean concentrations of Fe (0.6107 mg L^{-1}) and Mn (0.1835 mg L^{-1}) were observed, whereas Ni, Cu, Cd, Pb, and Zn were below detection limits. Fe and Mn exceeded Brazilian drinking water standards, indicating the water is unsuitable for direct consumption. Field observations and interviews confirmed that residents collect the water at the source and consume it without prior treatment, increasing exposure risks. The elevated Fe and Mn levels may be associated with natural geochemical features, such as the weathering of iron- and manganese-rich soils and rocks common in southwestern Bahia. However, anthropogenic contributions cannot be excluded due to nearby urban occupation, inadequate sanitation, surface runoff, and possible domestic effluent disposal, which may affect groundwater quality. Although essential at low levels, excess iron can intensify oxidative stress, and prolonged manganese exposure has been linked to neurological effects, particularly in vulnerable groups. Environmentally, these metals may accumulate in sediments and aquatic organisms, impairing ecosystem quality. The results underscore the need for continuous monitoring, hydrogeochemical studies to clarify contamination sources, and preventive measures to safeguard water resources and the health of communities relying on untreated spring water.



Trace Metals vs Legal Drinking Water Limits

Agradecimentos/Acknowledgments

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Assessment of the herbicidal potential of mangaba peel extract on Amaranthus retroflexus and Euphorbia hirta

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Palavras Chave:*Casca de Mangaba, Euphorbia hirta L, Amaranthus retroflexus, Bioherbicida, Alelopatia*

Highlights

Mangaba peel extract inhibited germination and early growth of target weed species, demonstrating herbicidal potential.

Resumo/Abstract

O uso intensivo de herbicidas tem favorecido o aumento da resistência de plantas daninhas, reduzindo a eficiência do controle químico e intensificando os impactos negativos sobre a produtividade agrícola. Nesse contexto, o presente estudo avaliou o potencial alelopático do extrato etanólico da casca de mangaba sobre a germinação e crescimento inicial de Amaranthus retroflexus (caruru-gigante) e Euphorbia hirta L. (santa luzia), espécies com elevado potencial competitivo, principalmente nos estádios iniciais de desenvolvimento das culturas, interferindo no crescimento das plantas cultivadas.

Os ensaios foram conduzidos com 600 sementes de cada espécie, distribuídas em placas de Petri e submetidas a diferentes concentrações do extrato etanólico da casca de mangaba (0 a 50 g L^{-1}). O experimento contou com quatro repetições de 25 sementes por concentração. As placas foram mantidas em germinadora, com temperatura controlada e programada ao longo do dia, e com fotoperíodo de 12 h, sendo avaliadas quanto à germinação e ao crescimento das partes aérea e radicular.

Os resultados demonstraram que, com o aumento da concentração do extrato, observou-se inibição da germinação de 90% e 100% para Amaranthus retroflexus e Euphorbia hirta L., respectivamente, na maior concentração avaliada. No caruru-gigante, o extrato também promoveu inibição do crescimento da parte aérea e radicular, evidenciando efeito alelopático significativo da casca de mangaba, sugerindo sua aplicação em estudos futuros voltados ao desenvolvimento de bioherbicidas de origem vegetal como alternativa ao uso de herbicidas sintéticos.

Agradecimentos/Acknowledgments

Os autores são gratos a CNPq pelo fomento da pesquisa.

AVALIAÇÃO DA REMOÇÃO DE HIDROCARBONETOS POLICÍCLICOS AROMÁTICOS (HPAS) EM SOLUÇÕES AQUOSAS POR ADSORÇÃO EM BIOCARVÃO DERIVADO DE GLICOSE

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Palavras Chave:*HPAs,Adsorção,Biocarvão,Carbono mesoporoso*

Highlights

Evaluation of PAHs removal from water. Adsorption on mesoporous carbon.

Resumo/Abstract

Os hidrocarbonetos policíclicos aromáticos (HPAs) são compostos orgânicos formados por processos naturais ou antropogênicos que apresentam alto potencial mutagênico e carcinogênico[1]. Este trabalho tem como objetivo avaliar a remoção de HPAs de matrizes aquosas por adsorção utilizando biocarvão derivado glicose[2] comparando sua eficiência frente ao carvão ativado comercial de ampla aplicação ambiental. O biocarvão estudado vem de um precursor renovável, possui estrutura mesoporosa bem definida e alta área superficial[2], o que o torna material de interesse para moléculas orgânicas aromáticas. Os experimentos de adsorção em carvão comercial (A) e biocarvão (B), foram realizados com soluções mix de acenafteno (ACE), pireno (PYR) e criseno (CRY), representando diferentes faixas de peso molecular, e com soluções contendo ACE. As massas de carvão utilizadas foram 6,25 mg, 8,45 mg e 100 mg conforme condições previamente otimizadas[3]. Nos ensaios com solução individual de ACE, observa-se remoções em torno de 50%. Para a solução mix, após tratamento prévio dos carvões com metanol e água (estufa por 24 horas a 120ºC), o carvão A apresentou remoção de 18% para o ACE e superior a 90% para PYR e CRY. Utilizando o carvão B, as remoções foram de 79% para ACE, 92% para PYR e 46% para CRY. Embora o carvão A tenha apresentado elevada remoção para PYR e CRY, sua eficiência foi limitada para ACE. O carvão B apresentou desempenho mais equilibrado e simultâneo para os 3 HPAs, característica relevante para aplicações ambientais de misturas complexas. Assim, a maior eficiência do carvão B na remoção de ACE, aliado ao uso de glicose como percursor renovável, está alinhado às demandas atuais de materiais a partir de fontes renováveis.

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Agradecimentos/Acknowledgments

Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) e ao Instituto Nacional de Tecnologia (INT)

Avaliação de Risco à Saúde Humana por Exposição ao Mercúrio e Determinação de Consumo Seguro de Peixes de Vila do Conde (Barcarena-PA)

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Palavras Chave:*Mercúrio,Vila do Conde,peixes,Subsistência,Risco à saúde.,Peixes*

Highlights

Mercury levels in subsistence fish from an Amazon industrial area; Habitat-driven differences in fish mercury bioaccumulation; Low health risk from fish consumption.

Resumo/Abstract

A região de Vila do Conde (Barcarena–PA) abriga um complexo industrial-portuário estratégico, voltado ao beneficiamento de alumina e à logística mineral. Essas atividades, associadas ao histórico de passivos ambientais e à mobilização de Hg na bauxita e nos solos locais, reforçam o monitoramento de Hg em peixes amazônicos, cujas concentrações variam conforme espécie e habitat [1,2]. O consumo de pescado é a principal via de exposição humana ao metilmercúrio, crítica para populações ribeirinhas. Este trabalho quantificou o Hg total (THg) em quatro espécies de peixes pertencentes a diferentes grupos tróficos e ecossistemas, visando avaliar o risco à saúde humana associado ao consumo dessas matrizes na região de Vila do Conde (Barcarena-PA).
A amostragem exploratória (n = 3 por espécie) foi realizada no Rio Pará (01°33'S, 48°45'O) para*Plagioscion squamosissimus*(Pescada-branca),*Pellona spp.*(Sarda) e*Astyanax sp.*(Piaba), e em igarapé adjacente para o*Heros efasciatus*(Acará-Severo). As amostras (26–560 g) foram acondicionadas em gelo para posterior análise. O músculo foi analisado em triplicata usando o analisador direto de mercúrio (DMA-80, Milestone) [3].
O maior teor médio de Hg foi encontrado no*H. efasciatus*, espécie onívora de igarapé (0,18 mg kg^{-1}). No Rio Pará, os teores foram inferiores variando de 0,07 mg kg^{-1} na*Pellona spp.*a 0,15 mg kg^{-1} para*A. sp.*e*P. squamosissimus*. As amostras estudadas não excederam os limites máximos estabelecidos pela legislação vigente (0,5 mg kg^{-1}para peixes não-predadores e 1,0 mg kg^{-1} para espécies predadoras) [4].
A avaliação de risco, baseada nos modelos de Felix et al. 2022 [3], considerou o Consumo Seguro (MSCQ) da USEPA, a Ingestão Semanal Estimada (EWI) e a Dose Semanal Tolerável Provisória (PTWI) da FAO/OMS [5]. Os resultados obtidos indicaram baixo risco toxicológico com THQ < 1,0 para adultos e EWI abaixo da dose tolerável, reforçando a necessidade de monitoramento contínuo, especialmente em ambientes de igarapé.

Agradecimentos/Acknowledgments

Os autores agradecem ao CNPq e a CAPES.

Avaliação do Uso de FeCl3 na Lixiviação de Ímãs Permanentes Obsoletos para Recuperação de Neodímio

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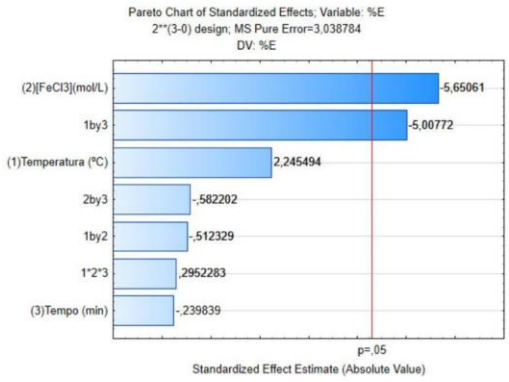
Palavras Chave:*Neodímio, Lixiviação, Elementos Terras raras, Recuperação, Valorização de resíduos*

Highlights

Concentração de FeCl3 e interação temperatura-tempo governam a lixiviação de Nd em ímãs permanentes obsoletos; Maior concentração de FeCl3 reduz porcentagem de extração de Nd por efeito de íon comum.

Resumo/Abstract

Este estudo avaliou a lixiviação de ímãs permanentes obsoletos (IPO) provenientes de HDs utilizando cloreto férrico (FeCl3) para recuperação de Nd. Um planejamento fatorial completo (2^k) com triplicata no ponto central foi aplicado para investigar o percentual de extração de Nd (%E) em função da temperatura, concentração de FeCl3 e tempo de lixiviação. A razão sólido-líquido foi mantida em 2,5% m/v, empregando soluções de FeCl3 preparadas em água com pH 1,00 ajustado com HCl. Determinação do metal foi realizada utilizando ICP-OES. Valores de %E variaram entre 75,74 e 90,93%, mostrando o potencial do FeCl3 como agente lixiviante. O diagrama de Pareto (Fig. 1) dos efeitos padronizados mostrou que, ao nível de confiança de 95% (p = 0,05), apenas dois termos influenciam significativamente o processo: a concentração de FeCl3 e a interação temperatura-tempo. A concentração do lixiviante apresentou o maior efeito absoluto, com sinal negativo, indicando que seu aumento reduz a %E. Esse comportamento pode ser atribuído ao elevado teor de ferro nos IPO (≈64% m/m), favorecendo efeito de íon comum e dificultando a solubilização das espécies da liga NdFeB. Temperatura e tempo, isoladamente, não foram significativos; contudo, sua interação apresentou elevada relevância estatística, indicando controle cinético acoplado do processo. Assim, o efeito da temperatura depende do tempo de reação e vice-versa, evidenciando que a otimização não deve ser feita de forma independente. As demais interações apresentaram influência desprezível dentro das faixas estudadas. Assim, o sistema é governado principalmente por um controle químico associado à concentração de $FeCl_3$ e por um controle cinético dependente da combinação temperatura-tempo. O baixo erro puro (3,038784), a reduzida falta de ajuste (≤0,758691) e o coeficiente de determinação elevado (R^2 = 0,96729) indicam bom ajuste experimental e sugerem a aplicabilidade de um modelo quadrático para otimização do processo.



*Pareto Chart of Standardized Effects; Variable: %E 2**(3-0) design; MS Pure Error-3,038784 DV: %E*

Agradecimentos/Acknowledgments

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Bauxite Beneficiation Routes for the Production of Value-Added Industrial Materials

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Palavras Chave:*Bauxite,mineral beneficiation,leaching,precipitation*

Highlights

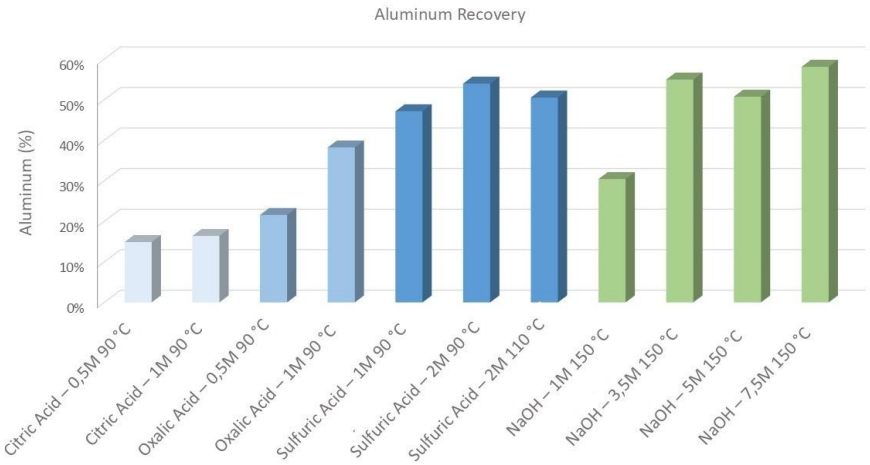
Alkaline digestion enabled selective aluminum recovery with minimal iron dissolution.
Sulfuric acid enhanced aluminum extraction but reduced selectivity.

Resumo/Abstract

Natural ores often contain impurities that restrict their direct industrial use, making beneficiation and purification routes essential to obtain higher-purity, value-added materials. Bauxite, mainly composed of aluminum hydroxides and silicates and associated with impurities such as iron oxides, silica, and titania, can have its industrial applicability significantly enhanced through selective purification strategies.

This study investigates acidic and alkaline routes for bauxite purification under different operational conditions, aiming at selective impurity removal and subsequent precipitation of aluminum hydroxide as a high-purity precursor. The ore was characterized by X-ray diffraction (XRD) and X-ray fluorescence (XRF). Acid leaching was performed using citric, oxalic, and sulfuric acids (0.5–2.0 mol L^{-1}) at 90–110 °C for 3 h, while alkaline digestion was carried out in a hydrothermal reactor using NaOH solutions (1.0–7.5 mol L^{-1}) at 150 °C for 4 h.

Mineralogical analysis identified gibbsite, kaolinite, anatase, goethite, and quartz as the main phases, with Al_2O_3 as the predominant component (74.3 wt%). Organic acids showed limited aluminum extraction, whereas sulfuric acid achieved higher aluminum recovery (59%) but with significant iron dissolution. In contrast, the alkaline route using 3.5 mol L^{-1} NaOH resulted in 55% aluminum recovery with minimal iron solubilization (0.2%), favoring the production of high-purity aluminum oxide. This condition was selected for aluminum hydroxide synthesis, currently under development.



Aluminum extraction yields obtained by different acidic and alkaline processes

Agradecimentos/Acknowledgments

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BEYOND MASS: ELEMENTAL COMPOSITION AND METEOROLOGICAL INFLUENCE ON PARTICULATE MATTER IN CATALAO-GO VS. CONAMA 506/2024 RESOLUTION.

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Palavras Chave:*Air Quality; EDXRF; Trace Elements; CONAMA 506/2024; Industrial Sources.*

Highlights

EDXRF linked PM to mining and industrial hubs in Catalão-GO. NE/N winds transported P, S and Nb from mining and fertilizer plants. CONAMA 506/2024 mass standards overlook specific toxic risks.

Resumo/Abstract

Resumo (Abstract): Air quality management in Brazil (CONAMA 506/2024) focuses on mass concentration (□g/m3), neglecting chemical composition. This study characterized PM10 and PM2.5 in Catalão-GO, a city influenced by carbonatite-hosted phosphate and pyrochlore mining (NE/N), fertilizer plants (NE), and an automotive hub (S). Samples were collected at UFCAT (colocated with INMET A034 station) and Downtown sites. PM mass concentration was determined by gravimetry, with values standardized to air volume corrected for atmospheric pressure and flow rate conditions. Elemental characterization was performed via EDXRF (Shimadzu EDX-7000) using the Fundamental Parameters method. To account for the thin-film nature of the samples, net intensities were calculated by subtracting blank fiberglass filter signals, eliminating matrix interference. Results showed PM10 peaks of 70.2 □g/m3 downtown. High net intensities of P and S (up to 2.50 cps) were linked to NE winds from mining/fertilizer activities. Nb tracers were identified above the blank baseline, consistent with local pyrochlore mineralogy (Cordeiro et al., 2011). High Fe downtown and S-winds suggest influence from automotive logistics and crustal resuspension. Correlation analysis confirmed that relative humidity (up to 79.46 %) reduced PM mass via wet deposition. The study concludes that meeting CONAMA mass standards is insufficient for public health, as specific toxic tracers from local geology and industry pose significant risks.

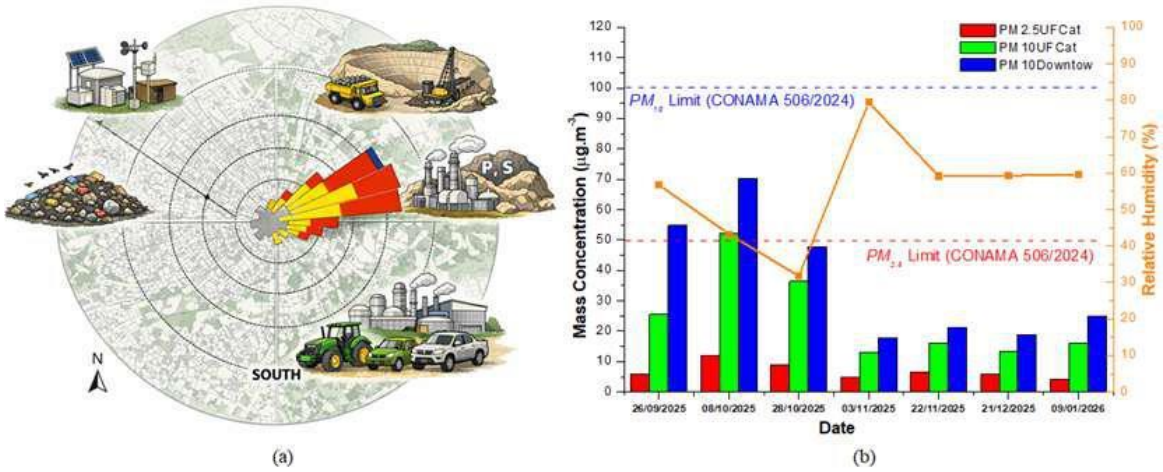


Fig.1: (a) Winds carry P,S,Nb,Fe/Cu to UFCAT. (b) PM–humidity shows wet deposition, CONAMA.

Agradecimentos/Acknowledgments

The authors thank UFCAT/IQ-UFCAT for infrastructure, the PIBIC/UFCAT program (scholarship for Ana Clara), and INMET for providing the meteorological data from station A034.

Bioactive C3-Functionalized 7-Hydroxycoumarins Against Citrus Phytopathogens

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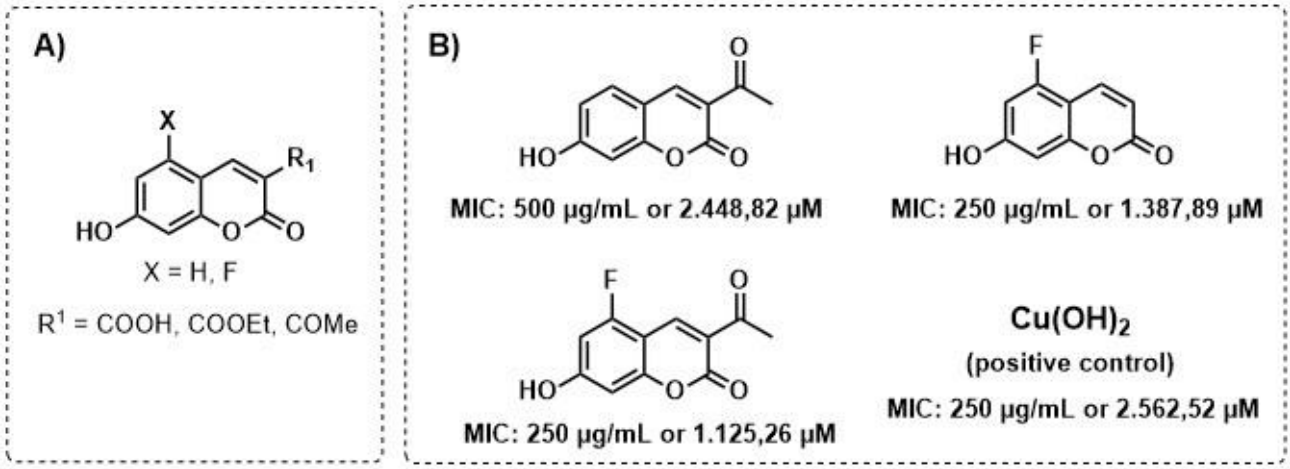
Palavras Chave:*Coumarins,Pesticides,Agriculture,Xanthomonas citri,Antibacterial*

Highlights

C-3 functionalized 7-hydroxycoumarins were synthesized and evaluated against*Xanthomonas citri*ssp. c*itri*. Three compounds exhibited MIC values lower than those of the positive control.

Resumo/Abstract

*Xanthomonas citri*ssp.*citri*are bacteria that affect*citrus*plants, causing citrus canker disease. Currently, the disease is controlled by applying copper-based bactericides; however, this use has resulted in the emergence of resistant strains and environmental and human health impacts. Because it affects a globally important fruit crop, this pathogen has been extensively studied in terms of disease management strategies, focusing on low-impact control and exclusion practices.[1] Coumarins are substances that have attracted attention for their diverse biological properties, including antibacterial activity. They are a class of secondary metabolites biosynthesized by plants that accumulate in response to infection by a variety of pathogens, including viruses, bacteria, and fungi.[2] Thus, the objective of this work is the development of C-3 Functionalized 7-Hydroxycoumarins, obtained mainly through Knoevenagel reactions (Figure 1A), and their evaluation for antibacterial activity against*Xanthomonascitri*ssp.*citri*through a microdilution assay in 96-well plates. The results for three compounds are promising, since the MIC values in μM against*Xanthomonas citri*ssp.*citri*are lower than the result presented by the positive control (Figure 1B).
[1]LIU, C.*et al.American Society for Microbiology***2025**,*16*, 1-17.
[2]Stringlis, I. A.*et al.Plant and Cell Physiology***2019**,*60*, 1405-1419.



C-3 functionalized 7-Hydroxycoumarins synthesized with MIC values lower than the positive control

Agradecimentos/Acknowledgments

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Biodegradable smart packaging based on starch and natural anthocyanins for food freshness monitoring

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Palavras Chave:*Colorimetric sensor,biopolymers,pH indicators,food quality,volatile compounds*

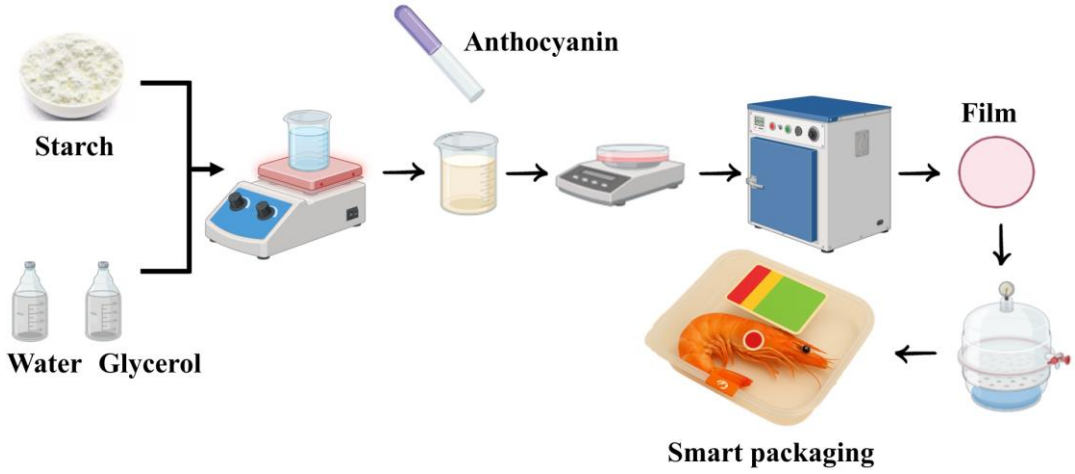
Highlights

Biodegradable smart films instantly reveal shrimp spoilage through visible color change;

Anthocyanin-based packaging enables real-time visual monitoring of seafood freshness

Resumo/Abstract

The demand for sustainable packaging capable of reducing plastic waste while monitoring food quality has driven the development of intelligent biodegradable materials. Anthocyanins are natural halochromic pigments sensitive to pH variations associated with the deterioration of protein-rich foods, standing out as promising freshness indicators. In this context, the present study developed and characterized biodegradable films based on Dioscorea sp. starch incorporated with anthocyanins for application as visual freshness indicators. The films were prepared by casting (4% starch, 1% glycerol) in the formulations F0 (0%), F5 (5%), F7.5 (7.5%), and F10 (10%) and evaluated in terms of physical and mechanical, structural, thermal, optical properties, and halochromic response. Thickness increased from 0.134 mm (F0) to 0.167 mm (F10). Extract-containing formulations showed higher moisture content and solubility, reflecting the hydrophilic nature of anthocyanins, while water activity remained between 0.54–0.60, below the threshold for bacterial growth. Water vapor permeability ranged from 1.66×10^{-9} (F0) to 1.91×10^{-9} $g \cdot m^{-1} \cdot s^{-1} \cdot Pa^{-1}$ (F10), associated with intermolecular reorganization induced by extract incorporation. The extract promoted progressive matrix plasticization, reducing tensile strength from 7.21 MPa (F0) to 0.62 MPa (F10) and increasing elongation at break from 14.58% to 62.99%. FTIR, XRD, and TGA analyses confirmed hydrogen-bond interactions, reduced crystallinity, and improved thermal stability. Films F5–F10 exhibited intense halochromic response across pH 2–13 (ΔE > 5). Exposure to ammonia induced rapid and visible color changes, demonstrating high sensitivity to volatile nitrogen compounds typical of protein food deterioration. It is concluded that the films show high potential as intelligent packaging for visual monitoring of food spoilage.



Smart packaging

Agradecimentos/Acknowledgments

The authors thank CAPES (Finance Code 001), INCT-CIMOL, PPGQ-UFPB, and NPE-LACOM for financial and technical support.

Biodegradation and phytotoxicity of pectin hydrogels in commercial soil

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Palavras Chave:*biodegradation,phytotoxicity,hydrogel,pectin*

Highlights

Biodegradation/phytotoxicity of hydrogels in soil were investigated. Germination index and relative root growth as parameters of study. Different sensitivities of vegetables in soils with hydrogel.

Resumo/Abstract

Pectin-based hydrogels were chemically synthesized in two steps. First, apple pectin purchased from Sigma-Aldrich® was modified with glycidyl methacrylate. Subsequently, the modified polysaccharide was copolymerized in the presence of acrylamide to form a three-dimensional hydrophilic cross-linked polymer network with high and adjustable water retention capacity. These biomaterials are potential matrices for soil conditioning and controlled nutrient release, contributing to the improvement of agricultural productivity. The degradation and phytotoxicity of the synthesized hydrogels were studied by burying approximately 0.10 g of biomaterial in 50 g of commercial soil at a depth of 3.0 cm. The system was monitored for 60 days at 20 °C under 50% humidity. The degradation process was preliminary evaluated by FTIR, TGA, and mass loss analysis. The soil pH decreased from 8.03 to 7.35 during the incubation period, whereas the electrical conductivity ranged from 430 to 939 µS cm^{-1}. The chemical oxygen demand increased from 151.6 to 437.6 mg L^{-1} when comparing the commercial soil before and after the hydrogel degradation process, indicating an increase in the organic matter content in the soil. Phytotoxicity assays were conducted via germination and root growth tests using lettuce (*Lactuca sativa*) and arugula (*Eruca sativa*) seeds over a period of 4 days. Based on the germination index (GI) and relative root growth (RRG), it was observed that the intermediate compounds formed during the degradation of the hydrogels generated moderate phytotoxicity in the studied plants. Overall, lettuce was more sensitive to phytotoxicity than arugula, as indicated by reductions in GI and RRG. In this sense, pectin-based hydrogels have demonstrated potential as matrices for agricultural applications due to their excellent biodegradability and very low phytotoxicity in commercial soils.

Agradecimentos/Acknowledgments

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Bioherbicide from Araticum and Mangaba Waste: A Green Approach to Control A. palmeri and M. pudica in Sugarcane Crops

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Palavras Chave:*QUÍMICA VERDE,BIOHERBICIDA,CANA-DE-AÇÚCAR,AMARANTHUS PALMERI,MIMOSA PUDICA*

Highlights

- Eco friendly bioherbicide from Cerrado fuit waste
- Total growth inhibition of A. palmeri by A. crassiflora
- Sustainable protection of sugarcane yield and ATR

Resumo/Abstract

A produção de cana-de-açúcar (Saccharum officinarum) enfrenta desafios devido à matocompetição de plantas invasoras como o caruru-gigante (Amaranthus palmeri) e a dorme-dorme (Mimosa pudica). Essas espécies reduzem o acúmulo de sacarose (ATR) e geram impurezas que prejudicam a fermentação do etanol. Diante da resistência a herbicidas sintéticos, a bioprospecção de espécies do Cerrado, como o araticum (Annona crassiflora) e a mangaba (Hancornia speciosa), torna-se fundamental. Este trabalho avalia como extratos etanólicos de suas cascas, ricos em acetogeninas e fenóis, influenciam a germinação e o vigor das plântulas, visando estender o Período Crítico de Prevenção da Interferência (PCPI).

O ensaio avaliou cem sementes de cada espécie em placas de Petri sob concentrações de 0 a 50 g L^{-1}. O material foi acondicionado em câmara de germinação (fotoperíodo de 12h) com inspeções diárias para quantificar a germinação e o alongamento da radícula e do hipocótilo.

Observou-se uma relação direta entre a atividade herbicida e a concentração dos extratos. Para a M. pudica tratada com mangaba, a inibição germinativa foi de 15,4%, com severa supressão no desenvolvimento da parte superior (29,1%) e da radícula (73,2%). Em contrapartida, a atividade sobre o A. palmeri com araticum foi total (100% de inibição) na dose de 50 g L^{-1}. Essa diferença sugere que as acetogeninas do araticum são mais prevalentes sobre a viabilidade das sementes, enquanto os compostos da mangaba retardam o vigor inicial, protegendo o ATR da cultura. Ademais, confirmou-se que a atividade bioherbicida da casca é tão expressiva quanto a de folhas e polpas descritas na literatura, validando o uso desse resíduo.

Conclui-se que as cascas de araticum e mangaba possuem alto potencial herbicida, agregando valor a resíduos descartados e oferecendo uma solução sustentável para o controle de invasoras que ameaçam a produtividade sucroenergética brasileira.

Chemical assessment of vermicomposting using Guarani and Brazilian cherry bagasse

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Palavras Chave:*Vermicomposting,Agro-industrial residues,Humification,Chemical stabilization,Tropical environments*

Highlights

Vermicomposting stabilizes tropical fruit bagasse in humid climates; Chemical indicators confirm humification and increased fertility; Guarany and Brazilian cherry bagasse yield stable vermicomposts.

Resumo/Abstract

Agro-industrial activities generate large volumes of organic waste throughout the production chain. Improper disposal can cause soil and water pollution and pose risks from a One Health perspective[1]. In Brazil, Guarani cherry (*Malpighia emarginata*) and Brazilian cherry (*Eugenia uniflora*) are widely processed for juice and frozen pulp, generating large amounts of bagasse as the main residue. Vermicomposting is an environmental technology that converts organic waste into a stabilized product with high agronomic potential through the action of earthworms and associated microorganisms[2]. This study evaluated the chemical dynamics of vermicomposting Guarani cherry (GC) and Brazilian cherry (BC) bagasse under the edaphoclimatic conditions of the Brazilian Atlantic Rainforest. The residues were mixed with buffalo manure and sawdust and inoculated with*Eisenia fetida*. Chemical monitoring included pH, electrical conductivity (EC), organic matter (OM), total organic carbon (TOC), and cation exchange capacity (CEC). OM decreased from 74.41% to 34.19% in BC and from 78.68% to 65.49% in GC, indicating organic matter transformation. CEC increased from 51.33 to 570.82 cmolc kg^{-1} in BC and from 88.41 to 540.14 cmolc kg^{-1} in GC, reflecting the formation of humified compounds. The pH increased from 4.88 to 5.54 in BC and decreased from 6.87 to 6.28 in GC, while EC remained low (<0.7 mS m^{-1}). Base saturation increased from 92.99% to 98.32% in BC and from 71.20% to 94.12% in GC, while aluminum saturation remained low (<2%). Despite differences in transformation intensity, both systems produced chemically stable vermicomposts. Vermicomposting efficiently converted both residues into materials with higher agronomic value, suitable for sustainable agricultural systems.

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Agradecimentos/Acknowledgments

The authors thank the Fundação de Amparo à Ciência e Tecnologia do Estado de Pernambuco (FACEPE) for the financial support provided through research grants awarded to M.R.Moraes (Process No. 1234456).

Chemical Modification of Buriti Fibers for the Formulation of Magnetic Adsorbents for Amoxicillin Removal

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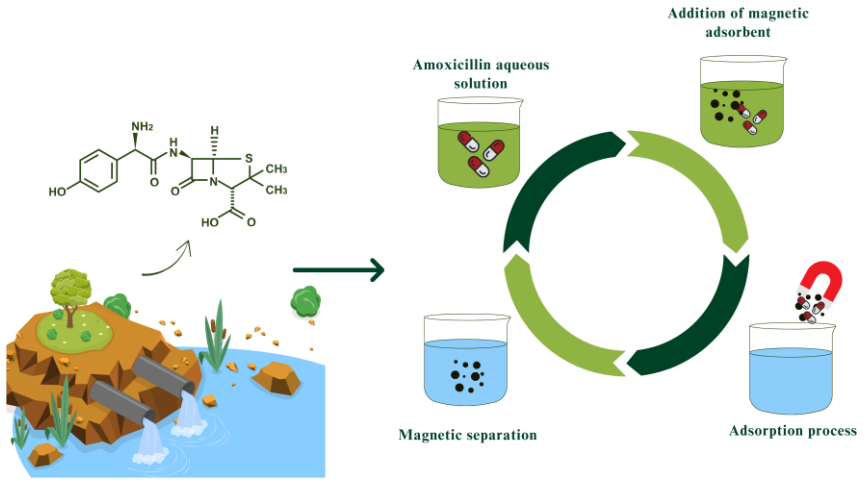
Palavras Chave:*Pharmaceutical contaminants,Lignocellulosic materials,Wastewater treatment,Plant-based waste*

Highlights

Development of a magnetic adsorbent from Amazonian residue; Chemical modification of Buriti fibers with alginate; Incorporation of $CuFe_2O_4$ for easy magnetic separation.

Resumo/Abstract

The increasing consumption of antibiotics in recent decades has intensified the release of these compounds into the environment, as many are not fully metabolized and reach water bodies through domestic and hospital effluents. Among emerging contaminants, amoxicillin stands out due to its frequent detection in surface waters and wastewater, as well as its potential to induce bacterial resistance. Given the limitations of conventional water treatment methods, adsorption has emerged as an efficient, sustainable, and economically viable alternative, especially when using low-cost materials from renewable sources. In this context, this study aimed to develop magnetic adsorbents through the chemical modification of Buriti fibers (*Mauritia flexuosa*), an abundant lignocellulosic residue in the Amazon region, combined with alginate and functionalized with copper ferrite ($CuFe_2O_4$) for the removal of amoxicillin in aqueous media. The magnetic oxide was synthesized using the proteic sol-gel method and incorporated into the polymeric matrix formed by Buriti fiber and alginate, resulting in a composite with a stable three-dimensional structure and magnetic properties suitable for solid–liquid separation. The materials were characterized by SEM-EDS, XRD, and nitrogen adsorption–desorption analyses, confirming ferrite incorporation and increased porosity. Batch adsorption assays were performed varying pH, adsorbent dosage, and initial drug concentration. The adsorbent was immersed in amoxicillin solutions (1–5 $\mu g \cdot mL^{-1}$). The $AlgMF@CuFe_2O_4$ composite showed q_e values close to 50 $\mu g \cdot g^{-1}$ in distilled water and slightly lower values (44–46 $\mu g \cdot g^{-1}$) in real water, indicating rapid adsorption kinetics and strong adsorbent–adsorbate interaction. The material also showed high adsorption efficiency and easy magnetic recovery, demonstrating its potential for environmental remediation.



Schematic representation of amoxicillin removal using a magnetic adsorbent and magnetic separation.

Chromium-Doped Magnetite Nanoparticles for Permanganate Ion Removal

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Palavras Chave:*CHROMIUM,MAGNETITE PERMANGANATE REMOVAL*

Highlights

- Iron mines with manganese contamination, as well as manganese mines, are found in various locations worldwide.
- Cr-dopen magnetite nanoparticles are a promising adsorbent for MnO4 - removal.

Resumo/Abstract

During manganese ore extraction, permanganate ions (MnO4 -) are released into water bodies, imparting an intense purple coloration that reduces light penetration, which can disrupt photosynthetic processes and negatively impact aquatic life. Additionally, their cytotoxic properties pose severe environmental and health risks. This study investigates the adsorption of MnO4 - onto Cr-doped magnetite nanoparticles (Cr-MNPs) as a potential remediation strategy for contaminated aqueous environments. Cr-MNPs and undoped magnetite nanoparticles were synthesized via the co-precipitation method and characterized using powder X-ray diffraction (XRD), revealing the presence of partially oxidized magnetite phases. X-ray photoelectron spectroscopy (XPS) analysis confirmed the high surface chemical purity of the materials, the presence of trivalent chromium at low concentrations, and the preservation of mixed Fe2+/Fe3+ surface species characteristic of magnetite, while revealing sample-dependent variations in surface oxygen species rather than a systematic increase in surface hydroxylation upon chromium incorporation. The adsorption process was evaluated by analyzing the effects of adsorbent dosage, contact time, and initial MnO4 - concentration, along with kinetic and isotherm modeling. Equilibrium was reached within 100 min, and experimental data were best described by the pseudo-second-order kinetic model and the Langmuir isotherm, indicating monolayer adsorption on a homogeneous surface. These findings demonstrate that Cr-MNPs are a promising adsorbent for MnO4 - removal, offering an efficient and sustainable solution for mitigating manganese contamination in aquatic environments, achieving a removal capacity of up to approximately 41 mg g-1.



Graphical abstract

Agradecimentos/Acknowledgments

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Chromium recovery from argentometric waste: didactic application and synthesis of nanostructured Cr_2O_3

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Palavras Chave:*Chromium,Waste recovery,Analytical chemistry,Nanoparticles,Sustainability*

Highlights

Sustainable management of Mohr argentometric titration waste.

Cr(VI) to Cr(III) reduction for $Cr(OH)_3$ recovery.

Recovered Cr converted to $Cr(NO_3)_3$ for teaching and to nanostructured Cr_2O_3 precursor.

Resumo/Abstract

Mohr argentometric titration generates residues that may contain toxic metal species, demanding treatment and reuse strategies consistent with green chemistry [1,2]. We developed a sequential protocol to recover chromium from such laboratory waste, adapting literature procedures for residues containing silver and chromium [2]. The waste was first treated with excess NaCl to precipitate Ag^+ quantitatively; the solid phase was separated by decantation for silver recovery. The supernatant was acidified with 6 M HCl until a yellow-to-orange shift, consistent with chromate (CrO_4^{2-}) to dichromate ($Cr_2O_7^{2-}$) conversion. Solid sodium thiosulfate was then added to reduce Cr(VI) to Cr(III), confirmed by an orange-to-green change and UV-Vis spectra [2]. This reduction is important because Cr(VI) is highly toxic and potentially carcinogenic, whereas Cr(III) is less toxic and nutritionally essential [1]. Next, the pH was adjusted to 10 with NaOH to precipitate $Cr(OH)_3$. After 48 h settling, the precipitate was filtered, dried (100 °C), and dissolved in 6 M HNO_3 to obtain $Cr(NO_3)_3$. The recovered salt was evaluated as a didactic reagent in semimicro qualitative analysis for group III (Cr^{3+}, Fe^{3+}, Al^{3+}, Zn^{2+}), showing practical viability for Analytical Chemistry teaching. Additionally, $Cr(OH)_3$ was used as a precursor for Cr_2O_3 nanoparticles by combining it with gelatin [3] and a plant extract [4], drying (90 °C), and calcining (500 °C), aiming at future electrochemical sensor applications. Overall, the procedure reduces stored waste volume, converts hazardous species into stable, reusable forms, and strengthens sustainable practices in chemistry education.

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Agradecimentos/Acknowledgments

FAPES (Mulheres na Ciências – Edital 21/2023, T.O.: 731/2024), LEA - UFES, Departamento de Química/CCE/UFES.

Clean urban mobility as a context for environmental education and chemistry teaching

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Palavras Chave:*public transport electrification; environmental education; basic education; CTS approach.*

Highlights

- Electric buses mitigate greenhouse gas emissions
- Clean mobility as a context for chemistry education
- Environmental education beyond a technological approach

Resumo/Abstract

Climate change has intensified over the years due to the growing emission of atmospheric pollutants, largely resulting from human activities. In this context, urban mobility has become one of the main contemporary environmental challenges, particularly because of the predominance of vehicles powered by fossil fuels. Consequently, many people rely on practical transportation options that emit significant amounts of greenhouse gases into the atmosphere each year, especially CO_2. In response to this issue, the municipality of Aracaju implemented a 100% electric public bus system aimed at reducing environmental impacts associated with greenhouse gas (GHG) emissions. This qualitative study, based on bibliographic and documentary research, presents a theoretical and reflective analysis of clean urban mobility as an educational context for environmental education and Chemistry teaching in basic education. By addressing real environmental problems and encouraging students to reflect on possible solutions—even through small actions—teachers can promote meaningful learning in which students become active participants in the construction of knowledge. This perspective also strengthens citizenship education by connecting Chemistry, Technology, and Society (CTS), allowing students to interpret chemical phenomena within real-world contexts. The study examines how the electrification of public transportation in Sergipe contributes to cleaner mobility and how environmental education can enhance school learning. The results highlight the relevance of implementing electric buses in Aracaju and empha their potential as an educational context for discussing environmental issues and contextualizing fundamental chemical concepts such as combustion reactions and stoichiometry. This approach promotes critical and civic-oriented learning and helps students understand the relationships between Chemistry, Technology, and Society while reflecting on solutions to current climate challenges.



Electric bus at a charging station.

Agradecimentos/Acknowledgments

IFS - Instituto Federal de Sergipe

Cobalt ferrite for the removal of Reactive Blue textile dye from aqueous solution

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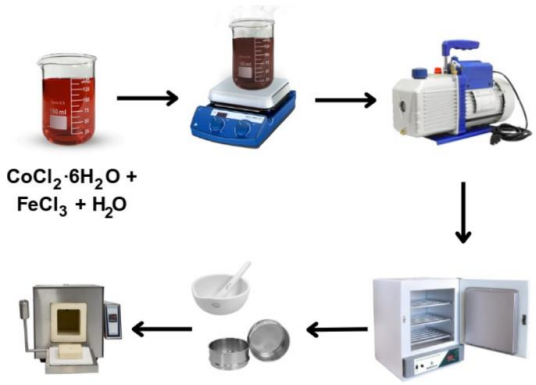
Palavras Chave:*Adsorption, Textile dyes, Magnetic ferrites*

Highlights

Magnetic cobalt ferrite rapidly removes Reactive Blue textile dye from water, combining fast adsorption, high capacity and favorable thermodynamics for efficient treatment of textile effluents.

Resumo/Abstract

The textile industry generates persistent colored effluents that impair aquatic ecosystems and hinder treatment by conventional methods. Adsorption has emerged as an efficient alternative. This study evaluates the efficiency of cobalt ferrite ($CoFe_2O_4$) for the removal of Reactive Blue textile dye from aqueous solution, assessing adsorption parameters, kinetics, equilibrium and thermodynamic aspects. $CoFe_2O_4$ was synthesized by alkaline coprecipitation followed by calcination. Surface characterization included determination of the pHpzc. Batch experiments evaluated the effects of adsorbent mass, pH, concentration, contact time, and temperature on dye removal. Data were fitted to PFO and PSO kinetic models and to the Langmuir and Freundlich isotherms, with determination of thermodynamic parameters. Surface characterization indicated a pHpzc of 6.3, where the positively charged surface favors interaction with anionic dye species. The pH effect confirmed strong electrostatic dependence, with maximum removal of 64% at pH 2 and a marked decrease under neutral and alkaline conditions. In mass-effect tests, removal remained nearly constant with increasing dose, whereas specific capacity decreased, highlighting 25 mg as the most cost-effective condition. Kinetic analysis showed that equilibrium was reached within 20 min, with best fit to the PSO model. qe values increased proportionally with initial concentration and were comparable to leading adsorbents reported in the literature. Equilibrium isotherms preferentially followed the Langmuir model, with a maximum capacity of 26 mg g^{-1}. Thermodynamic evaluation confirmed the spontaneous and endothermic nature of the process with increased entropy ($\Delta G°$ −31 to 37 kJ mol^{-1}; $\Delta H°$ +48 kJ mol^{-1}; $\Delta S°$ +238 J mol^{-1} K^{-1}). These results demonstrate the high potential of $CoFe_2O_4$ as an adsorbent for Reactive Blue dye removal, with prospects for optimization through surface modification or hybrid compositions.



Illustrative diagram of the cobalt ferrite nanoparticle synthesis route.

Agradecimentos/Acknowledgments

The authors acknowledge CAPES, FAPEMIG and CNPq for financial support and the Federal University of São João del-Rei (UFSJ) for institutional support.

Colorimetric sensor film with flavonoid rutin for determination of Cr(VI) in aqueous matrices.

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Palavras Chave:*Polymeric films,Colorimetric chemosensor,Ion detection,Environmental chemistry.*

Highlights

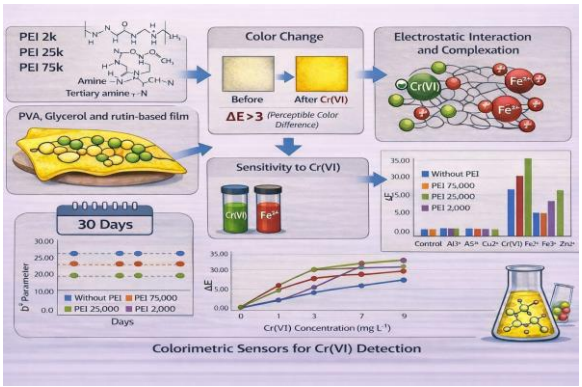
PVA- and rutin-based chemosensors modified with PEI.

Visual detection of Cr(VI) from 1 mg L^{-1}.

Colorimetric response stability for 30 days for films containing PEI of 25,000 and 75,000 g·mol^{-1}.

Resumo/Abstract

This study evaluated the effect of incorporating polyethyleneimine (PEI) with molar masses of 2,000, 25,000, and 75,000 g·mol^{-1} on the colorimetric response of films composed of poly(vinyl alcohol) (PVA), glycerol, and rutin, as well as on the stability of the analytical signal and selectivity toward different ions. The analytical response was evaluated in the concentration range of 0–3.5 mg L^{-1} of Cr(VI) under strongly acidic conditions (pH 1), in which the $HCrO_4^-$ species predominates. The addition of PEI significantly increased the color parameter b*, resulting in a more intense yellow coloration of the films, attributed to the reorganization of the polymeric matrix and the greater incorporation of rutin. Color variations were quantified using the CIELab system, in which ΔE (total color difference) was used as the analytical response parameter. ΔE values increased with increasing PEI molar mass and were perceptible to the naked eye even at a Cr(VI) concentration of 1 mg L^{-1}. The sensing mechanism is mainly attributed to electrostatic interactions between protonated amine groups of PEI and anionic Cr(VI) species, combined with ligand-to-metal charge transfer processes involving rutin. Although rutin is known to complex Cr(III), the results suggest that the observed response is predominantly governed by charge transfer interactions rather than by a redox process. Stability tests demonstrated that films containing PEI with molar masses of 25,000 and 75,000 g·mol^{-1} maintained a statistically stable colorimetric response for 30 days. Although partial discoloration was observed in aqueous medium, associated with rutin leaching, the persistence of sensor activity indicates that the fraction retained within the polymeric matrix is sufficient for analyte detection. Thus, the incorporation of PEI with higher molar masses significantly increases the sensitivity, selectivity, and robustness of the films, consolidating their potential as sensors for Cr(VI) detection.



PVA, glycerol and rutin-based chemosensor incorporated with PEI for Cr(VI) determination.

Agradecimentos/Acknowledgments

SBQ, UFOP, CAPES, CNPq, FAPEMIG.

Comparative study of silver purity recovered from analytical chemistry residues using sustainable methodology

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Palavras Chave:*Argentimetry,Residues,Silver,Sustainability,X-ray Diffraction*

Highlights

Silver recovered from Mohr/Volhard residues using a sustainable methodology.

The NaCl/NaOH/sucrose route produced FCC Ag and 95% purity for Mohr.

The method proved effective only for Mohr residues.

Resumo/Abstract

Argentometric titrations in volumetric analysis courses (Mohr and Volhard) generate silver-containing residues, increasing environmental liabilities and disposal costs. We evaluated Ag recovery from these residues via a low-cost, sustainable route consistent with green chemistry and circular-economy principles [1]. The procedure involved: (i) precipitating silver as AgCl with commercial NaCl; (ii) separating the supernatant; (iii) converting the precipitate to Ag_2O with NaOH under heating; (iv) “green” reduction of Ag_2O to Ag^0 using hydrolyzed sucrose; and (v) dissolution of Ag^0 in concentrated HNO_3 to produce $AgNO_3$ [1–3]. Metallic Ag was analyzed by X-ray diffraction (XRD) (Figure 1), and $AgNO_3$ purity was determined by titration with a NaCl standard solution. XRD distinguished the residues: for Mohr, a single crystalline Ag^0 phase (face-centered cubic; COD 9008459) with no secondary phases was obtained, consistent with 95% $AgNO_3$ purity. For Volhard, the diffractogram revealed a multiphase material dominated by AgSCN and AgBr with minor Ag^0, indicating incomplete conversion and yielding ~36% $AgNO_3$ purity. Because SCN^-/Br^- form stable, sparingly soluble silver salts, sucrose reduction is insufficient for Volhard residues and additional strategies (salt pre-treatment/conversion, modified reduction conditions, or alternative routes) are required to maximize recovery. Overall, the method is effective for Mohr residues, enabling $AgNO_3$ reuse in the laboratory and for nanoparticle synthesis and teaching experiments, whereas Volhard residues require further optimization.

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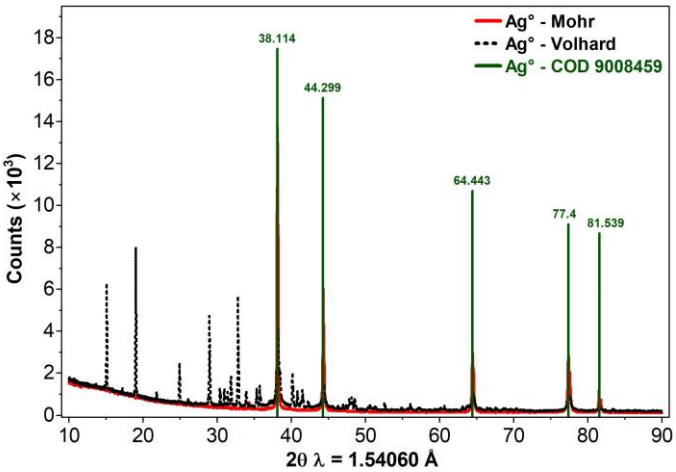


Figure 1. XRD: silver recovered from Mohr (red) and Volhard (black) residues.

Agradecimentos/Acknowledgments

Financial support from FAPES (Mulheres na Ciência – Call 21/2023, Grant 731/2024) is gratefully acknowledged. The authors also thank DQ/CCE/UFES and LDX-CCE/UFES for the XRD analyses (CT-Infra 01/2007-FINEP 0202/08).

Compositional changes of a spilled heavy oil under tropical conditions assessed by ESI(-) FT-ICR MS: A short-term laboratory simulation oil spill

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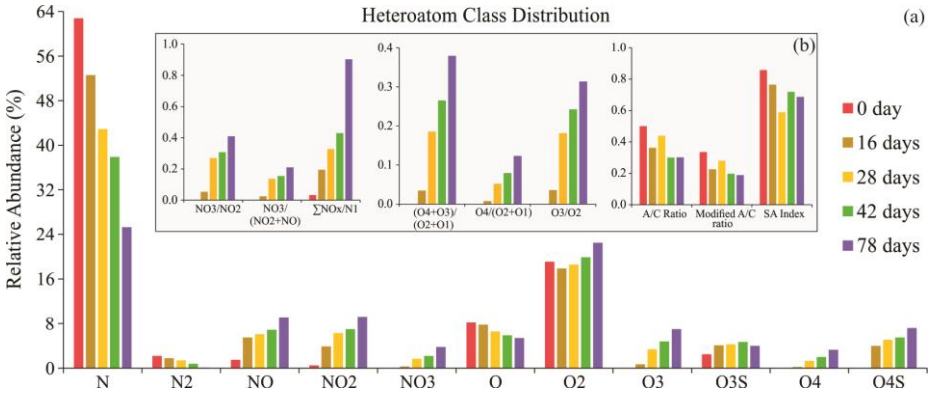
Palavras Chave:*Oil spill,Weathering,Tropical conditions,Biodegradation,Photooxidation*

Highlights

Weathering effects on spilled oils in tropical areas increase the abundance of oxygenated compounds, making the oils more toxic. Photooxidation and biodegradation are two of the weathering processes.

Resumo/Abstract

Once oil is released into the ocean, physical and chemical changes occur due to weathering processes, such as evaporation, photooxidation, and biodegradation. So, it is crucial to understand how these processes affect the chemical composition of petroleum spilled into the sea. In this context, this work aimed to assess compositional changes in polar compounds in a Brazilian oil during a short-term laboratory oil-spill simulation in seawater under tropical climate conditions, and to understand the main weathering processes affecting the oil composition. The oil spill simulation was performed from July to September 2024 at an experimental house in Macaé, Rio de Janeiro, using seawater collected from Pecado Beach, a 4.5 L aquarium, and 20 ºAPI crude oil. It was conducted for up to 78 days, with sample collections at 0, 16, 28, 42, and 78 days after the spill. The collected oil was assessed by a 7 T Bruker SolariX 2xR FT-ICR MS using an electrospray Ionization in negative mode [ESI(-)]. Over the course of the spill simulation, a significant increase in oxygenated classes with more than two oxygens, including NO_3, O_3S, O_4S, O_3, and O_4, is observed, likely due to photooxidation processes. The NO_3/NO_2, $NO_3/(NO + NO_2)$, $\sum NO_x/N_1$, $(O_4 + O_3)/(O_2 + O_1)$, $O_4/(O_2 + O_1)$, and O_3/O_2 heteroatom class ratios were applied, which increased over time, highlighting the effects of the photooxidation. In addition, the A/C ratio [DBE 1/(DBE 2 + 3 + 4)], modified A/C ratio [DBE 1/(DBE 2 + 3 + 4 + 5 + 6)] , and SA Index (DBE 1-6/O_2 class), which are based on the O_2 class, were calculated and decreased over time, disclosing that biodegradation was also a significant weathering process, with the increasing in the abundance of cyclic acids with DBE 2, 3, and 4. In conclusion, this work highlights the increase in the abundance of oxygenated compounds in spilled oils over time, increasing their toxicity, and discloses that biodegradation is also an effective process that contributes to these changes.



Class distribution for the spilled oils (a). Variation in the class ratios over spilled time (b).

Agradecimentos/Acknowledgments

We thank CNPq (DT II for Cruz, G.F.; 303424/2023-0), FAPERJ (APQ1 E-26/210.979/2024 for Martins, L.L.; CNE E-26/204.236/2024 and APQ1 E-26/210.146/2025 for Cruz, G.F), and CAPES for researcher funding and student grants.

Cumulative Impact of a Tannery and a Zinc Smelter on Surface Water Quality and Metal-Related Risks in the Paraibuna River, Minas Gerais, Brazil

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Palavras Chave:*Human health risk,Industrial contamination,Environmental risk assessment,Industrial effluents,Surface water contamination*

Highlights

Coexisting tannery and zinc smelter inputs shape trace metal contamination patterns and associated ecological and human health risks in a tropical river.

Resumo/Abstract

Surface waters downstream of industrial areas are frequently exposed to complex contaminant mixtures. This study evaluated the cumulative influence of a tannery and a zinc smelter on the Paraibuna River (MG, Brazil) through physicochemical characterization, trace metal determination, and integrated risk assessment.

Six surface water sampling sites were selected along the affected river reach, with triplicate collections. In situ measurements included pH, temperature, dissolved oxygen, and electrical conductivity. Major ions (Na^+, Ca^{2+}, Cl^-, SO_4^{2-}) were determined by standard methods (APHA, 2017). Trace metals (Cd, Cu, Zn, Mn, Pb, and total Cr) were quantified by ICP-OES.

Measured concentrations (mg L^{-1}) reached: Cd (0.012), Cu (0.045), Zn (0.38), Mn (0.62), Pb (0.009), and total Cr (0.07) at downstream sites. When compared to Brazilian surface water standards (CONAMA Resolution 357/2005), Cd exceeded the reference value (0.001 mg L^{-1}) by up to 12-fold, Mn (0.10 mg L^{-1}) by approximately 6-fold, and Zn (0.18 mg L^{-1}) by over 2-fold. Total Cr and Pb remained below the regulatory limits (0.05 mg L^{-1} for Cr and 0.01 mg L^{-1} for Pb), although they were retained as industrial tracers. Toxicological benchmarks for human risk assessment were based on USEPA reference doses (RfD).

Human health risk was assessed via ingestion pathway using Hazard Quotient (HQ) and Hazard Index (HI) calculations. HQ values >1 were observed for Cd and Mn at impacted sites, indicating potential non-carcinogenic risk. Ecological risk was evaluated using Risk Quotient (RQ = MEC/PNEC), revealing significant ecological risk for Cd (RQ >10) and moderate to high risk for Zn (RQ >2).

The results demonstrate that overlapping industrial discharges intensify trace metal contamination and pose measurable ecological and human health risks in the Paraibuna River, highlighting the need for integrated monitoring in mixed industrial corridors.

Agradecimentos/Acknowledgments

The present work was carried out with the support of the*Coordenação de Aperfeiçoamento de Pessoal de Nível Superior*(CAPES), Brazil – Finance Code 001.

Degradation of commercial plastic mulching films: a real-world approach.

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Palavras Chave:*LDPE,environmental aging,agriculture,microplastic,farmland*

Highlights

Four different colors of commercial mulching films were studied.

Hydrophilicity increased with time exposure.

Flexibility and rigidity showed opposite trends.

Resumo/Abstract

Mulching films made of low-density polyethylene (LDPE) are essential for global food security. The benefits include temperature and humidity control, weed suppression, and reduced pesticide use. However, mulching films are the primary source of terrestrial microplastics. In this context, four commercial LDPE mulching films with different colors (black, red, silver, and white) were exposed for 10 months at an experimental farm in Paulinia, São Paulo State, Brazil. The exposure area of each film was approximately 3.8 m². Samples of these films were collected monthly and analyzed using attenuated total reflectance Fourier-transform infrared (FTIR-ATR), gravimetry, mechanical testing, contact angle, differential scanning calorimetry (DSC), scanning electron microscope (SEM), and atomic force microscopy (AFM). The unaged films exhibited hydrophobic surface properties (>90°), but the degradation increases surface hydrophilicity. Contact angles decreased by 44, 49, 51, and 55% with aging for black, red, silver, and white films, respectively. The mechanical resistance was evaluated in two film extrusion orientations (transversal and longitudinal). In general, plastic's flexibility decreased, while the rigidity increased in both orientations. No clear trend in the dry weight of cleaned films over time was observed. However, the mass difference between the cleaned and raw films increased for black and red films but decreased for white and gray films. These results demonstrate that the dynamics of mulching degradation and biofilm formation are complex under environmental conditions, despite SEM images confirming the presence of biological elements and organic matter on the surface. These results assess mulching degradation under environmental conditions and can help with its appropriate management in the field.

Agradecimentos/Acknowledgments

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DEGRADATION OF SULFONAMIDES BY PHOTOCATALYTIC ACTIVATION OF HYDROGEN PEROXIDE BY WO3 UNDER UV-A IRRADIATION

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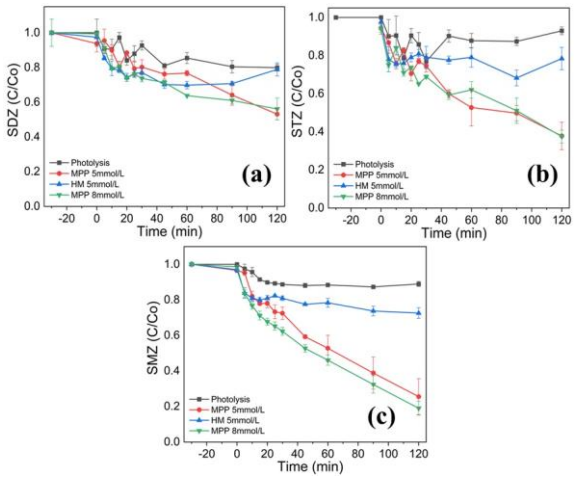
Palavras Chave:*Heterogeneous photocatalysis,Photochemical activation,Sulfanoamides*

Highlights

Peroxide photoactivation under UV-A ligth.
Degradation of a mixture of drugs.
Efficient production of hydroxyl and superoxide radicals.

Resumo/Abstract

Introduction: Sulfonamides are a class of antibiotics frequently found in different aqueous matrices due to their environmental persistence. Methodology: In this study, 0.125 g L-1 of WO3 produced by the polymeric precursor method (PPM) was used as a photoactivator of H2O2 to effect photocatalytic degradation under UV-A irradiation of a mixture (1 mg L-1 each) of sulfathiazole (STZ), sulfadiazine (SDZ), and sulfametazine (SMZ). To evaluate the effect of H2O2 on degradation, the study was conducted at oxidant concentrations of 5 or 8 mmol L-1. Results and discussion: After 60 min of UV-A irradiation, the photolysis of SDZ, STZ, and SMZ was less than 1%, while photocatalytic degradation was ≤ 7%, confirming their resistance to degradation. With the addition of H2O2 (5 mmol L-1), photolytic degradation increased, reaching 39%, 27%, and 26% for SDZ, STZ, and SMZ, respectively. On the other hand, the photocatalysis process resulted in higher efficiencies, with 62% for SDZ, 70% for STZ, and 82% for SMZ. These results indicate that WO3 and H2O2 contribute to oxidation reactions, promoting the formation of reactive species, such as HO• or O2•-, capable of degrading sulfonamides more effectively. As the degradation of SMZ was more pronounced, kinetic studies were performed using H2O2 concentrations of 5 mmol L^{-1} or 8 mmol L^{-1} for up to 120 min. The first-order rate constants for this antibiotic were k = 0.010 min^{-1} (R^2 = 0.989) and k = 0.012 min^{-1} (R^2 = 0.982), respectively. For photolysis, the maximum removal was 11% in 120 min, with no adequate fit for calculating the kinetic constant k. Conclusion: The combination of WO_3 and H_2O_2 under UV-A irradiation proved effective in the degradation of sulfonamides, exhibiting superior performance to photolysis and photocatalysis processes alone. SMZ showed greater susceptibility to treatment, and the kinetic data confirmed the efficiency of the system, with good fit to the first-order model.



Degradation profile of a mixture of SDZ, STZ, and SMZ (1 mgL-1 each) under different conditions.

Agradecimentos/Acknowledgments

FAPESP, CNPq, CAPES

Derramamentos de óleo no Atlântico Sul desde 2019: contribuição da química ambiental na avaliação da contaminação, risco à saúde e segurança alimentar

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Palavras Chave:*Risco à saúde; Contaminação costeira; Risco ambiental*

Highlights

O derramamento de óleo de 2019 impactou mais de 3.000 km da costa brasileira no Atlântico Sul.

Os derramamentos foram considerados um dos maiores impactos em regiões tropicais e na América do Sul.

Resumo/Abstract

A partir de 2019, praias ao longo da costa brasileira foram impactadas pela chegada de um volume estimado entre 5.000 e 12.500 m³ de material derivado de petróleo, disperso por mais de 3.000 km de litoral (Reddy et al., 2022). Embora a origem desse derramamento permaneça indefinida, novos episódios de menor magnitude continuaram sendo registrados nos anos subsequentes e ainda ocorrem de forma intermitente (Nascimento et al., 2025). Inicialmente, suspeitou-se que esses eventos estivessem associados ao derramamento de 2019; entretanto, análises geoquímicas posteriores demonstraram que os óleos apresentavam assinaturas químicas distintas, descartando uma relação direta entre eles (Azevedo et al., 2022; Nascimento et al., 2025). Apesar de os impactos ambientais associados a derramamentos de petróleo dependerem das características específicas de cada região afetada, as instituições brasileiras responderam de forma ampla e consistente aos desafios impostos por esse evento. Nos últimos anos, estima-se que entre 120 e 250 artigos científicos tenham sido publicados em periódicos nacionais e internacionais, abordando temas relacionados à química ambiental, em conjunto com ecotoxicologia, geoquímica do petróleo e geoquímica ambiental. Nesse contexto, a química ambiental consolidou-se como uma área estratégica no Brasil, deixando um importante legado científico e técnico. Sua contribuição envolveu o desenvolvimento e aprimoramento de métodos analíticos aplicados a diferentes matrizes ambientais, como água, sedimentos, organismos e o próprio petróleo. Esses estudos permitiram identificar, quantificar e interpretar contaminantes derivados do petróleo, incluindo HPAs, BTEXs e outros hidrocarbonetos. Além disso, o evento impulsionou significativamente a formação de recursos humanos especializados, fortalecendo a capacidade técnico-científica nacional na investigação de derramamentos de petróleo e seus impactos ambientais.

Agradecimentos/Acknowledgments

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Detection of MDMA and Other Classic Illicit Drugs in the Beberibe River (Recife-Olinda cities, Pernambuco, Brazil) During Carnival

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Palavras Chave:*1. Carnival,2. Environmental monitoring,3. Drugs of abuse,4. GC-MS,5. Emerging contaminants.*

Highlights

Multi-analyte GC-MS method for monitoring illicit drug. First detection of MDMA in Brazilian surface waters during the Carnival period. Cocaine was quantified in 100% of samples.

Resumo/Abstract

The presence of illicit drugs (ID) in aquatic environments has become an environmental concern because, after consumption, these substances are metabolized and excreted in urine, reaching wastewater treatment plants (WWTPs). Due to the inefficiency of conventional treatment processes, these compounds can be released into water bodies, contaminating riverbeds. The objective of this work was to collect and analyze surface waters from the Beberibe River in Recife-Olinda cities, Pernambuco state, Brazil. Nine samples were collected, six during the Carnival period (February 17-22, 2023), and three during a typical week (March 17-22, 2023). Samples were prepared using solid-phase extraction (SPE) and gas chromatography coupled to mass spectrometry (GC-MS) with a derivatization step, followed by validation according to ANSI/ASB 036 standards. Six analytes were investigated: cocaine (COC), benzoylecgonine (BE), cocaethylene (COE), methamphetamine (METH), 3,4-methylenedioxymethamphetamine (MDMA), and the cannabis metabolite 11-nor9carboxy-Δ9-tetrahydrocannabinol (THC-COOH). The method used 200 mL of surface water loaded into a Strata-X cartridge (200 mg, 6 mL), eluted with 3 mL of methanol followed by 3 mL of ethyl acetate. The method performance was evaluated by analyte recovery. (COC) and (BE) were detected in 100% of the samples, with the highest concentration of COC (887.8 ng L^{-1}) found on Carnival Saturday, coinciding with the “Galo da Madrugada” parade. MDMA was detected exclusively during Carnival (maximum of 19.3 ng L^{-1}), representing the first record in Brazilian rivers. THC-COOH showed a detection frequency of 83%, with high concentrations during Carnival (234.2 ng L^{-1}) and in the typical week (98.7 ng L^{-1}), indicating regular consumption. The Risk Quotient assessment indicated a moderate risk for cocaine and THC-COOH, highlighting the impact of seasonal anthropogenic inputs in the Beberibe River.

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Determination of anthropogenic particles in sardines (Sardinella brasiliensis) from the Baía de Todos os Santos

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Palavras Chave:*Anthropogenic particles,Microplastics,Sardines,Microscopy,Baía de Todos os Santos*

Highlights

Anthropogenic particles (APs) are chemical species resulting from human activities, including microplastics.

Studies have reported that sardines (*Sardina pilchardus*) serve as bioindicators of APs.

Resumo/Abstract

Anthropogenic particles (Aps) are chemical species resulting from human activities, including microplastics, fibers, rubber, and other microscopic industrial waste [1].
The identification of APs in the digestive tracts of fish has been used by ecologists to estimate pollution levels in marine ecosystems [1-3].
The standardized procedure for identifying Aps involves complete digestion of the fish's gastrointestinal tract with a 10% (w/v) KOH solution at 40 to 60 °C for 48 hours. Subsequently, filtration is performed using glass fiber filters, and the filters are analyzed using a stereomicroscope [2].
In this study, sardines (Sardinella brasiliensis) were obtained from fish markets that supplied fish caught in the Bay of All Saints. Fifty-one samples were analyzed, and thirty-five (68%) contained APs. A total of 80 APs were found, with an average of 2.29 ± 1.45 APs per sample and a median of 2. Of these APs, 75 were microparticles (94%) with s < 5 mm, and 5 were mesoparticles with s between 5 and 25 mm. The Fulton condition factor, which indicates a fish's nutritional status, was calculated and varied from 0.83 to 1.10, with a mean of 0.92 ± 0.06.
Spanish researchers analyzed 105 sardine (Sardina pilchardus) samples and observed a mean APs ingestion frequency of 15.24, with APs ingestion ranging from 0 to 3 APs per sample. They concluded that this fish can be used as a bioindicator of APs in marine environmental pollution [2].
Considering the results obtained with Spanish sardines [2] and those from previous research worldwide, it is concluded that Brazilian sardines can also serve as a bioindicator of APs in marine environment assessments [2,3].

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Agradecimentos/Acknowledgments

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in Coastal Ecosystems (COHAPPCO), i-COOP 2024 Call for CSIC (modality B). Reference: COOPB24025.

Development of a sample preparation method to determine the leaching of plastic additives from microplastics in water

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Palavras Chave:*plasticizers,flame retardants,OPFRs,PAEs*

Highlights

A sample preparation method was developed for application in MP leaching assays DLLME was suitable for evaluating the leaching of phthalates and organophosphate esters from plastic materials into wate

Resumo/Abstract

While a growing number of studies report the contamination of aquatic environments by microplastics (MPs), research correlating the influx of chemical additives leached from these particles to the aquatic environment remains scarce. Furthermore, there is a lack of standardized analytical methods for determining the lixiviation of these additives to water. Accordingly, the objective of this study was to evaluate the efficiency of three different extraction methods – liquid-liquid extraction (LLE), solid-phase extraction (SPE), and dispersive liquid-liquid microextraction (DLLME) – for aqueous sample preparation for the determination of phthalate and organophosphate esters (OPEs) using gas chromatography-mass spectrometry (GC-MS), to be applied to MP leaching experiments. The different methods were compared using aqueous samples spiked with 7 phthalates and 9 OPEs. Subsequently, they were applied in leaching assays conducted in a batch system using laboratory-produced MPs derived from various plastic materials (packaging, labels, and plastic bags), resulting on a mixture of different polymers (PP, PE and PET), which were ground in an industrial blender with dry ice and sieved to a range between 150 and 5000 µm. Figure 1 presents the recoveries. Although the LLE method showed good recovery results for all analytes, the lack of a pre-concentration step resulted in higher detection limits, preventing the detection of analytes in the leaching experiment. DLLME proved to be the most efficient regarding recovery values and detection limits, as well as in identifying a greater number of compounds leached from the MPs compared to the other methods, at levels ranging from 0.01 µg/g (TNBP) to 0.06 (TCIPP) µg/g. Additionally, given the ubiquitous nature of phthalates, DLLME offered advantages in controlling procedural blank contamination and significantly reducing solvent consumption. Therefore, the method proved advantageous in terms of sustainable analytical practices.

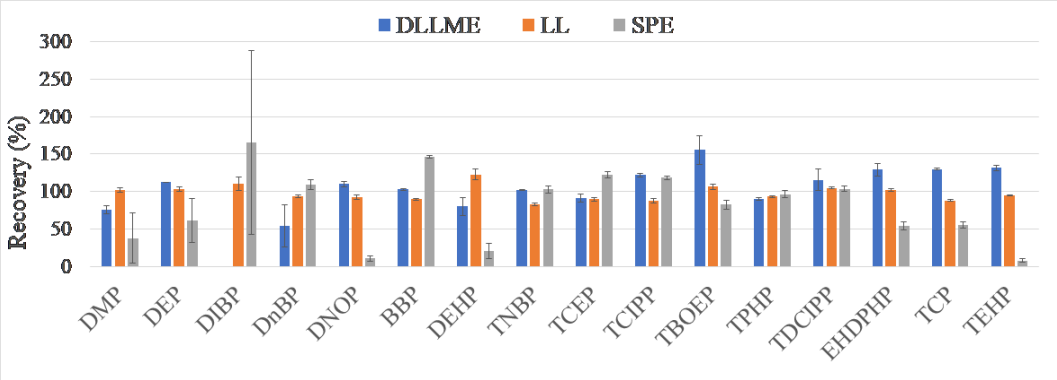


Figure 1 - Average recovery (n=3) of each analyte according to the tested extraction methods.

Agradecimentos/Acknowledgments

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Development of biodegradable intelligent packaging using biopolymers and anthocyanins from unconventional food plants (PANCs)

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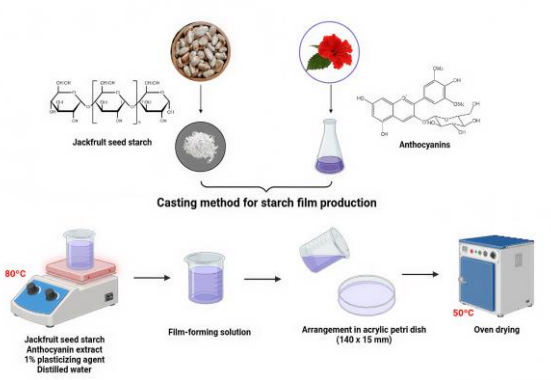
Palavras Chave:*Jackfruit seed starch, Anthocyanins, Intelligent packaging, Biodegradable films, Food quality monitoring,Jackfruit seed starch,Anthocyanins,Intelligent packaging,Biodegradable films,Food quality monitoring*

Highlights

The incorporation of anthocyanins provided high colorimetric sensitivity to pH changes and ammonia vapor. The smart packaging enabled visual monitoring of food quality and freshness.

Resumo/Abstract

The problem of environmental pollution caused by non-biodegradable petroleum-derived plastics, combined with the accumulation of agro-industrial residues, has driven the search for sustainable alternatives in the packaging industry. In this context, the development of bioplastics from renewable and underutilized resources emerges as a promising strategy to reduce the use of synthetic materials and promote the circular economy. Intelligent packaging based on biopolymers stands out for its ability to protect food while enabling the monitoring of quality and freshness during storage. Therefore, this study aimed to develop intelligent food packaging using jackfruit seed starch (Artocarpus heterophyllus) and anthocyanins extracted from vinagreira (Hibiscus acetosella), an unconventional food plant (PANC), as natural sensors. The methodology involved the extraction of the biopolymer and anthocyanins, followed by film preparation using the casting technique. The formulations were prepared with different concentrations of starch and extracts, 1% plasticizing agent, and distilled water, with the solution heated to 80 °C until starch gelatinization. The films were characterized in terms of tensile strength, thickness, morphology (Scanning Electron Microscopy), water solubility, water vapor permeability, thermal properties (Thermogravimetric Analysis and Differential Scanning Calorimetry), sensitivity to ammonia vapor, colorimetric response to pH, antioxidant activity, and soil biodegradability. The results indicated that the developed films exhibited suitable physicochemical, mechanical, and barrier properties, in addition to an efficient visual response to pH variations. It is concluded that the use of jackfruit seed starch and anthocyanins from Hibiscus acetosella represents a viable approach for the development of biodegradable intelligent packaging, adding value to underutilized raw materials and demonstrating potential for application as sustainable food packaging.



Biodegradable intelligent packaging

Agradecimentos/Acknowledgments

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Do resíduo ao adsorvente: uso do caroço de abacate na remoção de diuron e parationa metílica do meio aquoso.

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Palavras Chave:*Adsorvente,remoção,caroço de abacate,sustentável,agrotóxico.*

Highlights

A sustainable sorbent was obtained from avocado seed waste. Pesticides (diuron, methyl paration) removal from aqueous medium above 51.4% indicates high adsorption potential of avocado waste.

Resumo/Abstract

O caroço de abacate, frequentemente descartado, é um material lignocelulósico que apresenta grupos funcionais que favorecem sua utilização como adsorvente. Esses grupos podem promover interações químicas, como ligações de hidrogênio e interações eletrostáticas, com as moléculas de agrotóxicos, facilitando o processo de adsorção. Neste trabalho, o caroço de abacate foi avaliado como adsorvente alternativo para remover os agrotóxicos diuron (D) e parationa metílica (P) de meio aquoso, uma vez que esses compostos são tóxicos e estão associados a contaminação ambiental e ricos à saúde.
O adsorvente foi obtido a partir do caroço de abacate por processos de secagem, moagem, lavagem e peneiramento, sem necessidade de modificação química. Foram realizados ensaios de adsorção em batelada, analisando a influência da dose do adsorvente (10,00-25,00 g L-1), do tempo de contato (1-150 min) e da concentração dos agrotóxicos (2,00-38,00 mg L-1). A faixa de concentração foi definida considerando a solubilidade dos compostos em água.
Os resultados mostraram que o aumento da dose de adsorvente favoreceu a remoção dos agrotóxicos, com valores variando de 34,4% a 49,9% (D) e de 37,1% a 54,9% (P). O equilíbrio de adsorção foi estabelecido com 30 min para ambos os compostos, com remoção de 51,4% (D) e 55,0% (P). O modelo cinético de pseudo-primeira ordem apresentou o melhor ajuste, com R2= 0,9779 (D) e 0,9380 (P). Além disso, avaliou-se que, mesmo na maior concentração testada (38,00 mg L-1), foi removido 21,7% (D) e 31,9% (P). A capacidade máxima de adsorção foi de 0,7932 e 2,1195 mg g-1 para D e P, respectivamente.
Comparado a adsorventes descritos na literatura que requerem etapas de modificações química, como ativação com ZnCl2 para aumentar a eficiência, o material deste estudo tem a vantagem de ser obtido por processos simples, reforçando o seu potencial como um adsorvente alternativo e sustentável alinhados aos princípios da química verde.

Agradecimentos/Acknowledgments

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Dry biomass of Methylorubrum rhodesianum JABV-01 adsorbs potentially toxic elements from wastewater generated by electroplating processes

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Palavras Chave:*biosorption, bacterial biomass, hexavalent chromium, electroplating, bioremediation.*

Highlights

*Methylorubrum rhodesianum*JABV-01 biomass, with functional groups and rough morphology, removed Cr(VI), Ni, Zn, Fe and Cu from electroplating effluent, proving a low-cost sustainable bioadsorbent.

Resumo/Abstract

The present study aimed to characterize and evaluate the efficiency of residual bacterial biomass as an adsorbent for the removal of Cr(VI) from solution. The evaluated biomass consisted of cells of the bacterial strain*Methylorubrum rhodesianum*JABV-01, whose potential for the production of biomolecules of technological interest has been investigated by our research group. Adsorption experiments were carried out in batch mode using standard Cr(VI) solutions at 30 °C and 150 rpm, following a central composite rotational design (CCRD). The effects of pH, dry biomass dose of*Methylorubrumrhodesianum*JABV-01 (CB), contact time (t), and initial Cr(VI) concentration (C_0) on the Cr(VI) removal percentage (%R) were evaluated. The biomass exhibited a point of zero charge of 6.65±0.27 (at 30 °C), a rough, irregular, and granular morphology, functional groups such as hydroxyl and carbonyl, and carbon (C), nitrogen (N), and oxygen (O) as major components, in addition to trace amounts of other elements. Among the regression models applied to the response variable %R, the best fit was obtained for the simplified quadratic (stepwise) model (R^2 = 0.7558). Only the factors C_0 and CB significantly affected the Cr(VI) removal percentage. The optimal values of C_0, pH, CB, and t predicted from the response surface were 65.38 mg L^{-1}, 4.00, 19.36 g L^{-1}, and 90 min, respectively, resulting in a Cr(VI) removal percentage of 56.46±0.01%. Adsorption assays using synthetic wastewater and real electroplating industry wastewater, both containing Cr, Ni, Zn, Fe, and Cu, at pH 1.9, showed higher removal percentages for Cr (39.12±0.74%), Ni (72.96±0.72%), Zn (3.69±0.35%), and Fe (93.40±0.64%) in the synthetic effluent compared to the real effluent. For the real wastewater, at pH 3.71, the following removal percentages were obtained: Cr (31.93±1.27%), Ni (27.07±0.29%), Zn (21.45±0.47%), Fe (50.00±3.13%), and Cu (89.08±2.57%).

Agradecimentos/Acknowledgments

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Educação ambiental aplicada à pesquisa: aplicação de carvão derivado da pirólise de biomassa como adsorvente.

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Palavras Chave:*Milho,Biocarvão,Educação Ambiental,Extensão*

Highlights

Industrial effluents, especially toxic and persistent dyes, intensify water scarcity. Adsorption processes and biochars from agricultural residues offer a sustainable solution for water treatment.

Resumo/Abstract

A escassez de água potável e a intensificação da poluição hídrica por efluentes industriais configuram um grave problema ambiental e de saúde pública. Embora a água cubra grande parte do planeta, apenas uma fração mínima é acessível para consumo humano e ela é frequentemente contaminada por poluentes, especialmente corantes sintéticos, que afetam ecossistemas aquáticos e a saúde humana. Os corantes amplamente utilizados em setores industriais apresentam elevada estabilidade, toxicidade e baixa biodegradabilidade, dificultando sua remoção por métodos convencionais e favorecendo impactos como eutrofização e prejuízos à fotossíntese. Diante disso, o tratamento eficiente de efluentes, com destaque para processos de adsorção, torna-se essencial para o controle da poluição hídrica. Nesse cenário, a valorização de resíduos agrícolas lignocelulósicos, como o sabugo de milho, surge como alternativa sustentável alinhada à economia circular. A conversão desses resíduos por pirólise gera biocarvões com elevada área superficial e grupos funcionais, apresentando alto potencial para adsorção de contaminantes e menor impacto ambiental em comparação aos adsorventes convencionais.

Nosso projeto de extensão, além de produzir biocarvões a partir de sabugos de milho, promove a Educação Ambiental de alunos do ensino fundamental e médio de escolas públicas da região metropolitana do Rio de Janeiro, abordando o tratamento de água por adsorção de corantes em carvão ativado e seu reaproveitamento após a saturação. As ações são apoiadas por materiais de divulgação científica, como folders, banners, site institucional e conteúdos educativos divulgados no Instagram.



Representação da produção de biocarvões através da pirólise de sabugos de milho

Agradecimentos/Acknowledgments

Os autores deste projeto agradecem o apoio financeiro da CAPES e ao PPGQ-IME.

Environmental persistence of imidacloprid and tebuconazole in a water/sediment system after controlled contamination in mesocosms

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Palavras Chave:*Aquatic Environment,Sediment,Degradation,Pesticides,Microplastics*

Highlights

Tebuconazole has the slowest degradation.

The degradation product of imidaclopid, imidaclopid-urea, is found from the first days of the experiment.

Only tebuconazole was found in the sediment samples.

Resumo/Abstract

Emerging contaminants, such as pesticides and microplastics (MPs), pose risks to the aquatic environment. Due to its complexity, it is difficult to reproduce this environment; thus, mesocosms represent a balance between controlled and environmental conditions. The objective of this work was to study the degradation dynamics of the insecticide imidacloprid (IMI) and the fungicide tebuconazole (TEB) in aquatic mesocosm systems after controlled contamination, in the presence and absence of MPs. The mesocosms were divided into 5 treatments: control, isolated pesticides, and mixtures with and without MPs, classified as complex, intermediate, and less complex, according to the number of species and microphylls. Contamination was carried out according to the predicted environmental concentration: 46.68 µg L^{-1} for IMI, 32.26 µg L^{-1} for TEB, and 10 mg L^{-1} for MP per mesocosm. Water samples were analyzed by solid-phase extraction and sediment samples by solid-liquid extraction, subsequently quantified by liquid chromatography coupled to tandem mass spectrometry. The methods employed in both analyses were validated considering the following performance parameters: matrix effect, accuracy, precision, linearity, and limit of quantification. At the beginning of the experiment, IMI degraded more rapidly, forming IMI-urea at residual concentrations. Subsequently, the degradation rates were similar between the compounds, and after 120 days, the pesticides reached concentrations on the order of ng L^{-1}. The analytes didn't show sorption in the MP, which was confirmed by lab studies. Only TEB was found in the sediment samples, a result consistent with its physicochemical properties, indicating a greater affinity for the solid phase. This compound showed significant concentrations starting on the seventh day after contamination, reaching a peak after 14 days, followed by a decline in subsequent days, possibly due to its degradation into products incompatible with the method employed.

Evaluation of gunshot residue-related contamination in sport shooting ranges

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Palavras Chave:*Gunshot residue (GSR); Soil contamination; Toxic metals; Soil organic matter; Environmental pollution in.*

Highlights

Sport shooting alters soil geochemistry and toxic metal levels. Gunshot residues cause severe Pb contamination and alkalinization. Multivariate analysis shows a clear GSR gradient.

Resumo/Abstract

The rapid expansion of sport shooting ranges has raised environmental concerns within the One Health framework. Gunshot residues (GSR) contain potentially toxic elements such as Cr, Sb, As, and Pb, posing risks to human health and ecosystems due to their persistence in soils[1]. Soil organic matter (OM) plays a key role in regulating the mobility and retention of these contaminants. This study evaluated GSR-related contamination in soils from a sport shooting range in Recife, Pernambuco, Brazil. Samples were analyzed for organic matter, dry matter, pH, electrical conductivity, and elemental composition by X-ray fluorescence. Contamination was assessed using enrichment factor, geoaccumulation index, Pollution Load Index, and Combined Pollution Index. Clear chemical differences were observed between control and shooting range soils. pH values ranged from 5.60 to 10.27 and were consistently higher in shooting areas, indicating alkalinization associated with shooting practices[2]. Organic matter contents ranged from 1.36% to 4.82%, affecting metal retention and mobility[3]. Lead showed the highest concentrations, reaching 2763.76 mg kg^{-1}, with contamination indices indicating significant pollution, especially in surface soils. Principal component analysis revealed a clear contamination gradient associated with GSR. Overall, sport shooting activities significantly alter soil chemical properties and promote toxic metal accumulation.

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Evaluation of Landfill Leachate Generation and Treatment in the State of Rio de Janeiro between 2018 and 2025

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Palavras Chave:*Municipal solid waste management, Leachate treatment technologies, Environmental monitoring, Waste tracking and traceability,Municipal solid waste management,Leachate treatment technologies,Environmental monitoring,Waste tracking and traceability*

Highlights

Long-term assessment of landfill leachate management in Rio de Janeiro (2018–2025)
Over 99% of leachate treated by conventional wastewater treatment systems

Resumo/Abstract

Sanitary landfills are the main form of final disposal of municipal solid waste (MSW) in Brazil and constitute significant sources of landfill leachate, a highly complex effluent with considerable pollution potential. This study evaluates the generation and treatment routes of landfill leachate in the State of Rio de Janeiro from 2018 to 2025, based on annual data extracted from the Waste Transportation Manifest System (MTR) managed by the State Environmental Institute (INEA).

During the analyzed period, a total volume of approximately 3.47 million tons of leachate was recorded. Results indicate an almost exclusive predominance of wastewater treatment systems, accounting for about 99.2% of the total volume managed, while disposal in sanitary landfills represented approximately 0.8%. All other treatment routes, including transfer stations, re-refining, thermal treatment, recycling, composting, agricultural use, energy recovery, and other destinations, showed residual contributions, each individually accounting for less than 0.1% of the total.

The temporal analysis reveals a marked increase in leachate generation and destination from 2021 onward, with a peak in 2023, reflecting both the growth in disposed waste volumes and improvements in environmental control, traceability, and data recording systems. Overall, the findings demonstrate a strong dependence on conventional treatment technologies and limited diversification of leachate management strategies in the state.

It is concluded that, despite advances in monitoring and regulatory control, landfill leachate management in the State of Rio de Janeiro still requires investments in more integrated and efficient technological solutions, particularly under tropical climatic conditions and the high organic fraction of MSW.

From Molecules to Microplastics: Adsorption Behavior of Naphthalene and Naphthols on PET and PS

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Palavras Chave:*Adsorption,Microplastics,Polycyclic Aromatic Hydrocarbons (PAHs),Polyethylene Terephthalate (PET),Polystyrene (PS)*

Highlights

Naphthalene adsorption onto PET and PS followed pseudo-second-order kinetics.

PS showed higher adsorption than PET.

Naphthols showed no significant adsorption.

Salinity reduced naphthalene sorption.

Resumo/Abstract

The intense production and inadequate disposal of plastics have intensified the accumulation of microplastics (MPs) in aquatic environments, where they act as reactive surfaces capable of adsorbing organic contaminants. Among these contaminants, polycyclic aromatic hydrocarbons (PAHs) and their oxygenated derivatives are of particular concern.[1,2] This study investigated the adsorption of naphthalene, 1-naphthol, and 2-naphthol onto polyethylene terephthalate (PET) and polystyrene (PS) microplastics obtained from rigid post-consumer plastic cups. For both polymers, the materials were manually cut, mechanically ground, and sieved to obtain two MP size ranges (0.42–0.60 mm and <0.15 mm). Kinetic and thermodynamic behavior, as well as the effects of particle size and salinity, were evaluated. Kinetic experiments were conducted using 10 mg L^{-1} solutions for 180 min, and the data were fitted to pseudo-first-order and pseudo-second-order models. Equilibrium studies were performed at 5, 15, and 25 °C using naphthalene (1–30 mg L^{-1}) and naphthols (3–50 mg L^{-1}), for both MP size ranges, in distilled water and saline medium (NaCl 9 g L^{-1}), under agitation (90 rpm). Residual concentrations were determined by UV–Vis spectroscopy, and adsorption isotherms were adjusted to the BET model. Naphthalene adsorption onto PET and PS followed pseudo-second-order kinetics, with evidence of multilayer adsorption. Higher sorption capacity was observed for PS (Qm at 25 °C = 6.128). In contrast, 1-naphthol and 2-naphthol showed no significant adsorption under the evaluated conditions. Salinity reduced naphthalene adsorption onto both polymers but did not significantly affect naphthol sorption. These results indicate that the affinity of PET and PS for aromatic compounds strongly depends on contaminant hydrophobicity, suggesting a selective role of microplastics as PAH carriers in aquatic systems.

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[2] Environ. Sci.: Processes Impacts, 2025, 27, 849

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Fungal aerosols and volatile organic compounds in Indoor and Outdoor Air in Spain: Exploring Sampling and Analytical Methods

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Palavras Chave:*Viable fungal bioarosols,Coriolis µ sampler,Impactor sampler,VOCs,Fungi–VOC correlation*

Highlights

Impactor sampler recovered sixfold more viable fungi than Coriolis-µ, with highest levels outdoors. Hydrocarbons were predominant among VOCs at all sites. Viable fungi correlated only with Alcohol VOC

Resumo/Abstract

Fungi and volatile organic compounds (VOCs) can be constituents of, or associated with, the inhalable particulate fraction, contributing to human exposure in both indoor and outdoor environments[1,2]. This study quantified viable fungi and VOC concentrations in atmospheric samples collected in Madrid (Spain) and evaluated their statistical relationships, as well as compared fungal air-sampling methodologies. Samplings were conducted in different microenvironments at the CIEMAT–UCM campus: cafeteria, laboratory, storage area, and an outdoor site near a green area. Viable fungi were collected using a target air volume of 1 m^3 per replicate, comparing direct impaction onto culture medium (48 h incubation) with liquid sampling using a Coriolis-µ cyclone sampler. The Coriolis-µ showed low recovery efficiency, independent of the airflow rate (100 or 300 L min^{-1}), yielding approximately one-sixth of the colony-forming units obtained by the impactor; therefore, the impactor was selected for fungal quantification. Viable fungi concentrations ranged from 153±56 CFU m^{-3} (laboratory) to 789±215 CFU m^{-3} (outdoors), with intermediate levels observed in the cafeteria (248±75 CFU m^{-3}) and storage area (373±126 CFU m^{-3}). VOCs were collected using Tenax® tubes and analyzed by thermal desorption gas chromatography-mass spectrometry, quantifying hydrocarbons, alcohols, aldehydes, and siloxanes. Hydrocarbons were predominant at all sites (65.53-84.51 ppbv), while alcohols showed the greatest variability (15.61 ppbv to 63.85 ppbv). Aldehydes concentrations ranged from 0.99 to 1.74 ppbv and siloxanes from 0.05 to 0.16 ppbv. Statistical analyses indicated a significant correlation between viable fungal concentrations and alcohol VOCs, suggesting that this fraction may act as a chemical indicator of variability in viable fungal load in indoor and outdoor environments. 1.Can-Güven, E. Int. J. Environ. Sci. and Technol. 19, 7857–7868 (2022);2.Jia, C. et al. Atmos.Environ. 42, 2083-2100 (2008)

Agradecimentos/Acknowledgments

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Glitter killer: plasma electrolytic oxidation process as an alternative for microplastic remediation

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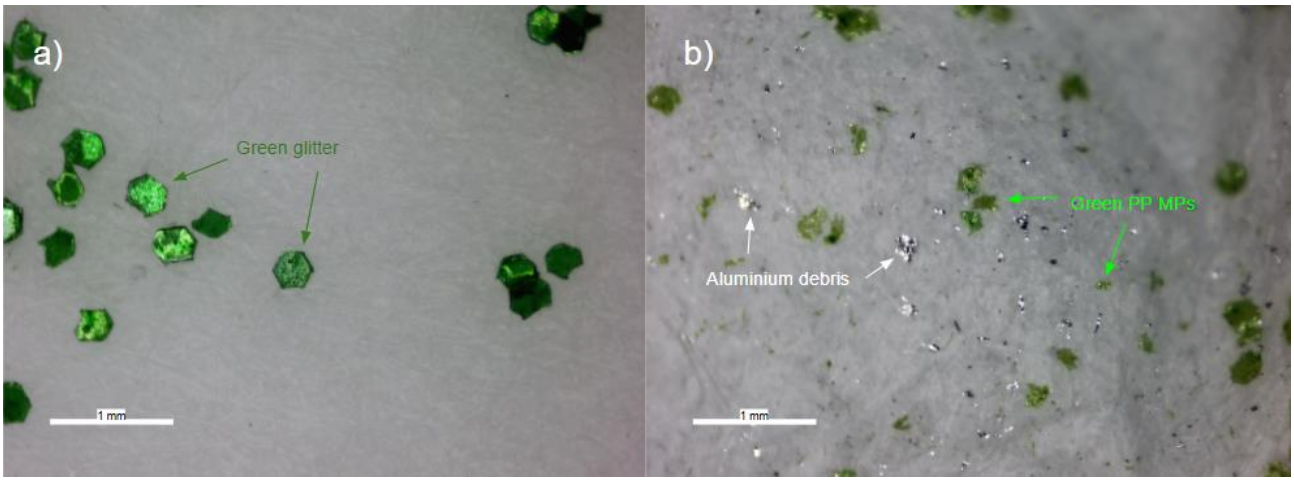
Palavras Chave:*Remediation,PEO,microplastics,pollution*

Highlights

Plasma Electrolytic Oxidation has the potential to remediate microplastics. After 90 minutes of processing, the polypropylene of the glitter fragmented, revealing the aluminium layer.

Resumo/Abstract

Microplastic pollution (MPs) is a contemporary and global problem. Several measures are being planned and implemented to address this issue. Despite the effects already observed, advances in understanding the impacts of microplastics and the actions taken to prevent their leakage into the environment, the remediation of this contaminant remains a challenge.
This work aims to evaluate the potential of the Plasma Electrolytic Oxidation (PEO) process for the remediation of microplastics in water. Controlled essays were conducted using a homemade AC/DC power source, with aluminum electrodes (98.7%) immersed in a 0.075 mol/L sodium silicate electrolytic stirred solution containing approximately 0.01 g of glitter for different durations (30, 90, 150, and 300 minutes), with the current density set at 20 mA/cm² and an applied voltage of approximately 400 V. The microplastics, the electrodes, and the electrolyte were analyzed using optical microscopy, SEM, FT-IR and DLS. Optical microscopy evidenced the fragmentation of polypropylene into smaller fragments and the detachment of the aluminum film layer that composes the glitter (attached Figure 1). Overall, the results of this work indicate microplastic degradation, with potential migration of degradation products into the aqueous medium and onto the electrode surface.



Optical microscopy images of: (a) control PP and (b) PP after PEO treatment for 90 minutes

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Halogen and sulfur profile in seaweed from Brazilian Northeast

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Palavras Chave:*Seaweed; MIC; Halogens; Sulfur*

Highlights

The halogen and sulfur content was quantified for the first time in seaweed samples from the Northeast Brazil.

A high variation in halogen and sulfur content was observed with seasonality.

Resumo/Abstract

Halogen and sulfur data in macroalgae are scarce, being focused on temperate and polar species, with tropical macroalgae underrepresented. Halogens play an important role in the defense metabolism of macroalgae, and the sulfur present in the structural components of macroalgae physiological function. The sample preparation using Microwave-induced combustion (MIC) becomes viable halogen analysis due to decompose complex matrix and form non-volatile species. The combination of MIC and Ion Chromatography (IC) makes it possible to determine halogens and sulfur in a single run. In this work, halogens (Br, Cl, F, I) and sulfur were quantified in macroalgae species from Ceara State. For sample preparation, around 500 mg of macroalgae samples were weighed onto LPDE films, which were heat-sealed and placed on quartz holders with filter paper discs moistened with 50 µL of 6 mol L^{-1} NH_4NO_3 then placed in quartz vessels containing 6 mL of 150 mmol L^{-1} NH_4OH absorber solution, closed and pressurized with O_2 with 20 bar. The MIC procedure was carried out with an irradiation program of 1400 W for 5 min, and 20 min for cooling. After decomposition, the samples were diluted and analyzed by IC. The results showed a high variation of concentration of the analytes with seasonality. Higher levels of halogens were observed in the brown macroalgae*Sargassum vulgare*(1597 ± 84 mg kg^{-1} for iodine and 827 ± 10 mg kg^{-1} for bromine) and in the red macroalgae*Bryothamnion triquetrum*(67940 ± 3045 mg kg^{-1} for chlorine) during the rainy season. All results for fluorine were below the quantification limits (7 mg L^{-1}). Moreover, sulfur levels increased during the dry season. The high halogen content found compared with polar and temperate seaweed suggests that abiotic stressors and ecological pressures in tropical zones may increase the production of halogenated secondary metabolites. These findings provide essential data for the nutritional and industrial application of marine macroalgae biomass.

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Industrial Effluents and Chemical Pollution in the Sergipe River Estuary, Northeastern Brazil

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Palavras Chave:*Industrial effluents; Water quality; Heavy metals; Estuarine pollution; Environmental chemistry*

Highlights

- Industrial effluents drive chemical degradation of the Sergipe River
- Heavy metals accumulate due to estuarine hydrodynamics
- Risks to aquatic ecosystems and human health persist

Resumo/Abstract

Industrial effluents are recognized as important sources of chemical contamination in aquatic environments, particularly in estuarine systems where hydrodynamic processes can influence the transport and accumulation of pollutants. This study analyzes information reported in scientific studies and institutional monitoring reports on the water quality of the Sergipe River estuary, located in Northeastern Brazil, with emphasis on the influence of industrial activities and other anthropogenic pressures between 2021 and 2025. The research was conducted through a systematic review of scientific articles and technical reports, focusing on physicochemical parameters and environmental indicators such as dissolved oxygen, turbidity, biochemical oxygen demand (BOD), nutrients, and heavy metals.

The analyzed studies and environmental monitoring reports indicate water quality alterations in sections influenced by urban and industrial activities, particularly in areas near the metropolitan region of Aracaju. Some reports describe elevated BOD values and increased turbidity, suggesting the presence of significant organic loads in the aquatic system. In addition to industrial discharges, untreated domestic sewage has also been identified as an important factor contributing to the deterioration of water quality, mainly through the increase of organic matter and nutrient inputs in the estuarine environment.

The reviewed studies also report the presence of metals such as lead, cadmium, and mercury, indicating possible contamination associated with industrial activities. In estuarine environments, the interaction between river flow and tidal dynamics can favor the accumulation and remobilization of these contaminants in sediments, which may prolong environmental exposure and affect aquatic organisms. Overall, the analyzed information highlights the importance of continuous environmental monitoring and improvements in wastewater management, contributing to a better understanding of poll

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Instituto Federal de Sergipe - IFS

INFLUENCE OF THE ORDER OF DEPROTEINIZATION AND DEMINERALIZATION STEPS ON CHITIN EXTRACTION FROM CRAB SHELLS

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Palavras Chave:*Chitin,Crab shell,Deproteinization,Demineralization*

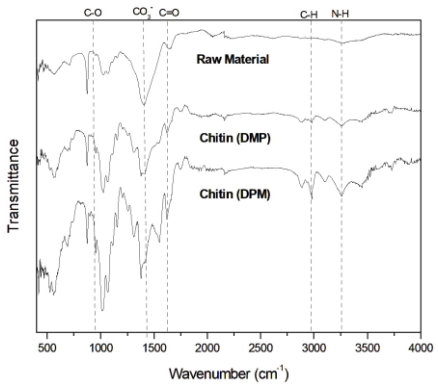
Highlights

Crab shells as a renewable biomass source for chitin production.

Processing sequence directly influences chitin extraction efficiency and valorization of crustacean residues.

Resumo/Abstract

Chitin is an abundant biopolymer widely explored as a functional material, commonly obtained from crustacean waste. Its extraction process generally involves deproteinization and demineralization steps, whose sequence can directly affect extraction efficiency, purity, and material quality. In this study, the influence of processing sequence on chitin extraction from crab shells was investigated. Two routes were compared: deproteinization followed by demineralization (DPM) and the reverse sequence, demineralization followed by deproteinization (DMP), under similar experimental conditions. Cooked crab shells were washed, oven-dried, ground, and sieved. In the deproteinization step, the resulting powder was treated with a NaOH solution, while in the demineralization step it was treated with an HCl solution. Three cycles were performed for each route (DPM and DMP). Ash content analysis indicated higher demineralization efficiency when using the DPM route (1.2%) compared to the DMP route (3.7%), relative to the ash content of the dried shell (61.3%). The efficiency of protein and carbonate removal was evaluated by FTIR spectroscopy. The increase in characteristic chitin absorption bands was investigated, including O–H/N–H stretching (3260 cm^{-1}), amide I (1620 cm^{-1}), and polysaccharide-related vibrations (950 cm^{-1}). Likewise, the disappearance of the characteristic carbonate peak (1400 cm^{-1}) and the significant reduction of protein-associated bands (1650 cm^{-1}) were observed. Overall, greater efficiency in both deproteinization and demineralization was achieved using the DPM route. Therefore, the results indicate that performing three cycles of the DPM route leads to the production of purer chitin from residual crab shells, favoring the development of more efficient and sustainable routes for chitin extraction from biomass.



FTIR spectra of chitin samples obtained after the demineralization and deproteinization processes.

Agradecimentos/Acknowledgments

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Interaction of the insecticide Ethion with copper(II) ions: implications in the aquatic environment.

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Palavras Chave:*Ethion,Copper(II) Complexes,Electrochemistry,Organophosphate,Pesticides*

Highlights

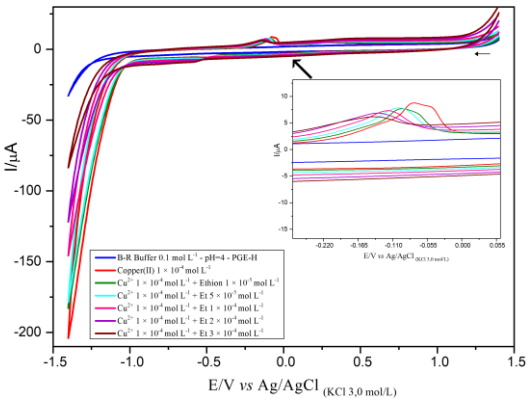
Electrochemical study of the organophosphate Ethion.

Interaction of the pesticide Ethion with copper(II) metal ion.

Investigation of the interaction between ethion and copper in natural waters.

Resumo/Abstract

Ethion (Et) is an organophosphate insecticide and acaricide that is banned in countries of the European Union but authorized in Brazil for application on citrus fruits, nuts, and cotton. It is also used in veterinary medicine as a cattle bath for tick control. This insecticide is highly toxic to fish and aquatic arthropods and exhibits moderate toxicity (class II) to humans. Therefore, its interaction with other elements present in the environment, such as metals, may amplify its harmful effects on living organisms. Copper is a naturally occurring element and is essential to living organisms; however, in excess, Cu^{2+} ions can cause neurodegenerative disorders. In this context, this study investigates the interaction between Ethion and copper(II) ions using electrode. The supporting electrolyte was 0.1 mol L^{-1} Britton–Robinson (B–R) buffer (pH 4.0). Using a mechanical pencil graphite electrode (PGE) as the working electrode, Cu^{2+} showed a reduction process at −0.048 V and an oxidation process at −0.062 V, characteristic of a quasi-reversible system. After the addition of Et to the Cu^{2+} solution at [Cu^{2+}:Et] ratios of 1:0.1, 1:0.5, 1:1, 1:2, and 1:3, a shift of the peaks toward more negative potentials was observed (−0.127 V and −0.531 V for oxidation and reduction, respectively). Furthermore, this study emphasizes identification using more sustainable techniques, enabling the indirect analysis of Et with an electrode constructed from mechanical pencil graphite. This approach represents an innovation in the study of this insecticide, as the literature primarily reports the use of mercury electrodes to obtain its voltammetric signal.



Copper(II) 0.0001 mol L^{-1} in B-R solution (0.1 mol L^{-1}) with additions of aliquots of Ethion

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Invisible Players in the Atmosphere: Fungal Aerosols and Volatile Organic Compounds

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Palavras Chave:*Fungal bioaerosols,Volatile Organic Compounds,Fungi–VOC correlation,Air quality*

Highlights

Fungal bioaerosols and volatile organic compounds constitute chemically and biologically active fractions of the atmosphere.

Bioaerosols and VOC are key indicators of air quality and human exposure.

Resumo/Abstract

Atmospheric pollution is a major environmental risk to human health, driven in part by the coexistence of chemically and biologically active airborne components in environment. Among these, bioaerosols and volatile organic compounds (VOC) are relevant to air quality assessment. Bioaerosols constitute a biologically active fraction of particulate matter, including fungi, viruses, pollen and metabolites. Their abundance and composition depend on emission sources, such as soil, vegetation and agricultural activities, and environmental factors, including temperature, relative humidity and wind.[1] These particles can contribute to infections and respiratory problems, induce oxidative stress and chronic inflammation and often carry bioactive compounds, like endotoxins.[1,2] They may also influence meteorological processes and enable long-range transport of pathogens, promoting the spread of diseases.[1] VOC (benzene, toluene and formaldehyde) are highly volatile compounds emitted from anthropic and natural sources in indoor and outdoor environments. These compounds contribute to secondary pollutant formation and can cause respiratory and neurological effects, as well as carcinogenic, teratogenic, or mutagenic outcomes.[2] Despite their importance, bioaerosol characterization remains analytically challenging, as different sampling and detection methods yield distinct information and detection limits.[3] Culture-based approaches quantify viable microorganisms, while molecular techniques and chemical biomarkers provide complementary insights into sources and variability. In this context, the combined assessment of viable fungal bioaerosols and VOC provides a broader understanding of airborne chemical and biological interactions. Because both fractions vary with emission sources, environmental conditions, and analytical strategies, their integrated interpretation improves air quality evaluation and underscores the critical role of methodological choices in atmospheric monitoring.

Agradecimentos/Acknowledgments

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Liga Mineral, an Interactive Comic Book for Schools.

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Palavras Chave:*Sustainability,Enviroment,Schools,Comics,Comic Book*

Highlights

Liga Mineral is a comic book that embarks on its first exciting adventure, teaching sustainable mining practices and environmental care through fun stories and interactive games for young students.

Resumo/Abstract

Science communication plays a central role in bridging the gap between academic research and society, especially in complex and socially sensitive areas such as mining. In this context, narrative and visual strategies are important tools for mediating scientific knowledge, contributing to the construction of scientific literacy and expanding public access to science. This work presents the development of the comic book Liga Mineral as a science communication resource conceived within the scope of the 1000 Futuros Cientistas Extension Program (1000FC), with the aim of communicating research developed by the Rede Mineral Escalab to non-specialized audiences. The comic book was developed from an interdisciplinary process involving Visual Arts students, Chemistry undergraduates, and researchers in the mining field, adopting principles of educational design and public communication of science. The narrative addresses topics related to mining, tailings treatment, water quality, filtration processes, and sustainability, articulating scientific concepts with socio-environmental and territorial issues in an accessible and contextualized way.
The material was designed for use in science outreach activities, such as fairs, educational workshops, extension events, and science popularization activities. The analysis of the creation process concludes that the narrative and visual language favors the understanding of complex scientific content, stimulating public interest and expanding the potential for dialogue between science, territory, and society.
The results highlight the role of comics as relevant instruments for science outreach and education in formal and non-formal spaces, reinforcing the contribution of Visual Arts in the translation of scientific knowledge. The work also highlights the potential of the material as an educational resource to be explored in future stages, strengthening the interface between university extension, mining research, and science education.



The main characters in the comic book Liga Mineral are students from public schools.

Agradecimentos/Acknowledgments

The authors are grateful to the Federal University Of Minas Gerais (UFMG) and the project 1000 Futuros Cientistas (1000FC) for funding and support.

Material funcional em gel para liberação controlada de coagulantes e floculantes aplicado ao tratamento de efluentes industriais

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Palavras Chave:*Materiais funcionais,Tratamento de efluentes,Coagulação e floculação,Liberação controlada,Materiais funcionais]*

Highlights

Gel-based material developed for controlled release of coagulant and flocculant agents; Improved stability and efficiency in industrial wastewater treatment;

Resumo/Abstract

Industrial wastewater treatment remains a significant challenge in Environmental Chemistry, particularly due to the complexity of liquid matrices and the strong dependence of coagulation and flocculation processes on operational conditions. In this context, this work presents the development and evaluation of a functional gel-based material designed to act as a controlled-release system for coagulant and flocculant agents applied to industrial wastewater treatment.

The material was synthesized from a polymeric network capable of modulating surface charge and promoting particle aggregation through a combination of electrostatic neutralization and polymer bridging mechanisms. Physicochemical characterization involved spectroscopic and thermal techniques, as well as zeta potential analysis, enabling correlations to be established between structure, thermal stability, and interfacial behavior of the system.

Laboratory-scale experiments were carried out using real industrial effluent in order to evaluate clarification efficiency and material robustness under different operational conditions. The results demonstrated superior performance of the gel-based system compared to conventional formulations, evidenced by higher turbidity removal efficiency and greater process stability. These outcomes are attributed to the gradual release of active agents and improved dispersion of the material in the aqueous medium.

Overall, the developed material exhibits strong potential for industrial-scale application, considering its compatibility with existing treatment systems and its ability to reduce variations associated with chemical dosing. This work highlights how industry-driven technological demands can foster the development of functional materials, contributing to more efficient and sustainable solutions for industrial wastewater treatment.

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Metal-doped porous carbon from polystyrene recycling waste as adsorbent of emerging contaminants from water

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Palavras Chave:*carbonates; plastic reuse; pharmaceuticals; dyes; water treatment*

Highlights

Polystyrene waste was applied as a carbon precursor to produce the adsorbent.

The potassium-doped carbon showed better performance towards hydrophobic contaminants.

Resumo/Abstract

In adsorption studies, the hipercrosslinked polymer (HCP) has been investigated by simple one-pot synthesis and production of materials with high surface area. To produce HCP, several precursors can be applied, including plastic waste. This work aimed to produce a mesoporous carbon by using HCP from polystyrene waste and dope it through one-pot pyrolysis with carbonates.

The carbons (H-MPC@Li, H-MPC@Na, and H-MPC@K) produced usingLi_2CO_3, Na_2CO_3, and K_2CO_3, respectively, were characterized and applied as adsorbents of pharmaceuticals, dyes, and surfactants. The N_2 physisorption showed type I isotherm to H-MPC@K, and type IV isotherm to H-MPC@Li and H-MPC@Na. The BET analysis showed surface area of 293.4 m^2/g, 291.9 m^2/g, and 936 m^2/g to H-MPC@Li, H-MPC@Na, and H-MPC@K, respectively. The chemical analysis showed that H-MPC@K was more hydrophobic and less negatively charged than H-MPC@Li and H-MPC@Na.

The adsorption of several contaminants was evaluated through the material H-MPC@K, which showed the best performance in removing levofloxacin, ketoprofen, and basic orange 2, probably associated with the more hydrophobic characteristics, aromatic rings and p-p interactions. In sequence these contaminants were evaluated by the other materials. Levofloxacin was best removed by H-MPC@K, compared to the pristine HCP, H-MPC@Li, and H-MPC@Na. To the contaminant basic orange 2, H-MPC@Li showed best adsorption, compared to the other materials. Both materials (H-MPC@Li and H-MPC@K) showed pseudo-second order kinetics, and the isothermal studies showed better fitting to Freundlich and Redlich-Peterson to H-MPC@K and H-MPC@Li, respectively.

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Microplastic contamination in the Iriri River: implications for protected forest regions

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Palavras Chave:*Emerging Pollutants, microplastic, freshwater, Amazon forest.*

Highlights

Characterization and quantification of microplastics.

Presence of microplastics in freshwater.

Plastic pollution in rivers.

Resumo/Abstract

The Iriri River is an important tributary of the Xingu River, and after about 35 km from its source, located in the Serra do Cachimbo, Altamira, PA, it enters the Panará Indigenous Land. Because of fishing and the use of water for human consumption, for example, this stretch is of great importance to this community, where about 750 people live, distributed across 7 villages. The objective of this study was to analyze the presence of microplastics (MPs) in different sections of this river, considering mainly the distance from the border of the Indigenous Land and the proximity of the villages, in order to verify the resilience of the forest in accumulating MPs and the contribution of daily activities as a source of contamination. Fifteen samples were collected at different points of the Iriri River between Aug 2023 and Jul 2025, using a 64 µm mesh net over 3 min of collection. The sampled water volume was calculated using a flowmeter. The extraction of MPs consisted of removing organic matter by digestion with Fenton's reagent (acidified Fe(II) and H_2O_2). Subsequently, density separation was performed with a supersaturated NaI solution (ρ = 1.6 g cm^{-3}). The identification of MPs was carried out through an initial screening under a stereomicroscope (Leica S6D), with magnifications of 4x to 10x, allowing the physical characterization of MPs in terms of shape (fragment, fiber, sphere, film, or pellet) and color. The chemical characterization (in process) will be conducted by Fourier-transform infrared microspectroscopy (µFTIR, LUMOS II Bruker), using an FPA (Focal Plane Array) detector. Fragments and fibers were the most particles identified, mostly white or transparent. The level of contamination is much lower compared to urban areas. The samples collected near to the villages were the most contaminated, indicating a potential source of input of MPs to the river. The seasonality influences are under evaluation.

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Novel sweet potato starch-based aerogel containing graphene oxide applied in the removal of safranin dye

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Palavras Chave:*Adsorption, Sustainable Starch, Nanoadsorbent, Water treatment*

Highlights

Sustainable starch/graphene oxide aerogel efficiently removes safranin from water, evaluating pH, dosage, contact time, and temperature. DFT and post-adsorption analyses will clarify removal mechanism

Resumo/Abstract

Water contamination by synthetic dyes is a major environmental issue due to their high stability, persistence in aquatic ecosystems, and potential toxic effects on organisms and human health. The continuous discharge of industrial effluents compromises water quality, highlighting the need for efficient and sustainable treatment technologies. In this study, a sustainable aerogel based on sweet potato starch incorporated with graphene oxide (SPS@GO) was developed for the removal of safranin dye from aqueous solutions. The adsorption performance of SPS@GO was evaluated through batch experiments by investigating the effects of solution pH, adsorbent mass, contact time, and temperature. The results showed that pH plays a decisive role, with higher removal efficiencies under near-neutral and alkaline conditions due to favorable electrostatic interactions. An optimal adsorbent mass was identified, indicating saturation of active sites at higher dosages. Contact time experiments revealed that adsorption equilibrium was reached after approximately 12 h, consistent with diffusion limitations within the porous structure. Temperature studies indicated that adsorption is favored at ambient conditions, with reduced efficiency at higher temperatures. Kinetic analyses demonstrated that the adsorption process follows the pseudo-second-order model, suggesting that the rate is governed by interactions between safranin molecules and active sites on the aerogel surface. In addition, studies on adsorbent–adsorbate interactions based on density functional theory and post-adsorption characterizations are being conducted to clarify removal mechanisms, and future studies will focus on regeneration cycles and performance in real wastewater matrices, aiming to strengthen its application in sustainable water treatment. Overall, the SPS@GO aerogel demonstrated excellent performance for the removal of safranin, combining high adsorption capacity with environmental sustainability.



SPS@GO aerogel

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Optimizing the sorption and desorption of sulfadiazine in pectin hydrogel

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Palavras Chave:*sorption, sulfadiazine, pectin hydrogel,Sorption,sulfadiazine,pectin hydrogel*

Highlights

- Pectin hydrogel for water remediation;
- Optimized removal of sulfadiazine at pH 3.0;
- Process with high regeneration and reuse capacity.

Resumo/Abstract

The optimization of sulfadiazine (SDZ) sorption in pectin hydrogel (HPEC) and subsequent desorption studies revealed the ideal conditions for removing this drug from aqueous media. The general methodology consisted of contacting 50 mg of HPEC with 50 mL of SDZ solution (18 mg L^{-1}) under controlled stirring. The maximum removal efficiency (11.73 mg g^{-1}) was achieved at pH 3.0. The zero loading point (ZLP) of the material was 4.7, indicating a positively charged surface below this value. Sorption at acidic pH is favored by the intense formation of hydrogen bonds between pectin and the cationic forms of SDZ. At pH above 7, the sorption capacity decreases significantly due to electrostatic repulsion between the HPEC surface and the drug, both of which are negatively charged. The adsorbative equilibrium was reached in approximately 60 min. The pseudo-second-order kinetic model showed the best fit (R^2 = 0.9487), suggesting that the limiting mechanism involves chemisorption with electron sharing between the active sites and the pollutant. Increasing the initial concentration of SDZ increased the adsorption capacity. The Freundlich model best described the process (R^2=0.9991), indicating a heterogeneous surface and the formation of multilayer adsorption. The increase in temperature resulted in lower removal efficiency, characterizing sorption as an exothermic process. To evaluate SDZ recovery, saturated samples were subjected to solvent extraction (ethanol, HCl, and water) under stirring at 100 rpm. The results indicated that the most favorable media for desorption were 0.001 mol L^{-1} HCl (74.8%) and the aqueous medium at a temperature of 40 °C (71.7%), demonstrating the potential for regeneration and sustainable reuse of the adsorbent.

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Oxidative potential of aerosol collected in São Paulo during biomass burning events as an indicator of health risk

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Palavras Chave:*Particulate matter, Oxidative potential, DTT assay, Biomass burning, Vehicular traffic,Particulate matter,Oxidative potential,DTT assay,Biomass burning,Vehicular traffic*

Highlights

Potential oxidative evaluate the impact of particulate matter for human health.
Determination of organic and inorganic species.
Strong correlations between OPDTT and species related to burning biomass.

Resumo/Abstract

Oxidative potential (OP) has been widely used as a metric to assess the health risk associated with atmospheric particulate matter, because it directly relates to the ability of particles to generate reactive oxygen species (ROS) and induce oxidative stress, a mechanism associated with the development of diseases such as cancer. In this study, the OP of $PM_{2.5}$ collected in the city of São Paulo during the winter of 2024 (n =37) was evaluated, a period characterized by the highest number of wildfire hotspots ever recorded in the state, and influenced by air masses coming from the Amazon region. The chemical characterization of the aerosol included PAH, oxy and nitro PAH, determined by gas chromatography, monosaccharides and ions determined by ion chromatography, and metals by inductively coupled plasma mass spectrometry. The oxidative potential determined by dithiothreitol assay (OPDTT) showed a mean value of 2 nmol min^{-1} m^{-3}, consistent with elevated levels reported in urban environments impacted by combustion sources. The maximum value of 5 nmol min^{-1} m^{-3} was observed on the day with the highest wildfire activity and $PM_{2.5}$ concentration (82 µg m^{-3}). OPDTT exhibited statistically significant Spermann correlations with biomass burning tracers, such as potassium, levoglucosan, retene and rubidium, highlighting the central role of this source in the redox activity of $PM_{2.5}$. In addition, strong correlations were observed between OPDTT and the total concentration of PAH, oxy and nitro-PAH, indicating the contribution of aromatic organic compounds and derivatives to ROS generation. Correlations with traffic related metals (Cu, Cd, Mn, Pb and Zn) also highlight the influence of vehicular emissions on $PM_{2.5}$ toxicity. Overall, these results demonstrate that elevated OP levels in São Paulo are predominantly driven by primary combustion sources, particularly biomass burning and vehicular traffic, emphasizing the potential impacts of these activities on human health.

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Pesticide Use in Corn Farming and Environmental Impacts in Northeastern Brazil: A Case Study in Simão Dias, Sergipe

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Palavras Chave:*Pesticides,Environmental chemistry,Corn farming,Human health,Water contamination*

Highlights

- Intensive pesticide use linked to corn farming in Northeastern Brazil
- Environmental contamination risks to soil and water resources
- Impacts on biodiversity and human health in rural communities

Resumo/Abstract

The intensive use of pesticides is a central issue in environmental chemistry due to its implications for soil, water, and ecosystem integrity. This study evaluates pesticide use in the municipality of Simão Dias, located in the agreste region of Sergipe, Brazil, a major corn-producing area strongly influenced by seasonal agricultural demand associated with regional cultural festivities. A qualitative case study approach was adopted, combining bibliographic and documentary research with analysis of secondary data from official institutional sources. The results indicate that the expansion of corn farming has been accompanied by increased application of agrochemicals, contributing to potential contamination of soil and surface water, degradation of permanent preservation areas, and risks to local biodiversity. Evidence of pesticide drift, including aerial spraying, highlights the vulnerability of riparian zones and water resources. From an environmental chemistry perspective, the study emphasizes the behavior, dispersion, and persistence of pesticide residues in environmental compartments and their implications for human exposure, particularly among rural workers and nearby populations. The findings reveal contradictions between agricultural productivity and environmental sustainability, reinforcing the need for improved monitoring, environmental risk assessment, and the adoption of safer and more sustainable pest management strategies. This case study contributes to broader discussions on pesticide regulation, environmental governance, and sustainable agriculture in semi-arid and transitional ecosystems.

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Instituto Federal de Sergipe

POTENTIALLY TOXIC METALS IN AQUACULTURE SYSTEMS

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Palavras Chave:*Aquaculture, Water quality, Potentially toxic metals, Accumulation index*

Highlights

Diagnosis of the input-output of potentially toxic metals in a fish farming enterprise: Accumulation Index and Seasonal Variation.

Resumo/Abstract

In this study, the dynamics of potentially toxic metals (Al, Ba, Fe, Mn, and Zn) in water quality were evaluated in an intensive fish farming system located in western Paraná, Brazil, with a focus on their contribution to the accumulation and output of these metals to the environment. Sampling was conducted during the four seasons of 2024/25 at different points within the facility, including water intake points (river abstraction), culture tanks, settling tanks, and the water outlet point (discharge to the environment). Potentially toxic metals such as Al, Ba, Fe, Mn, and Zn were analyzed using inductively coupled plasma optical emission spectrometry (ICP-OES) and flame atomic absorption spectrometry (FAAS). Figure 1 presents the seasonal variation profiles of Al, Fe, and Mn concentrations at different points of the fish farming system.

Based on the measured concentrations, pre-concentration (PF) and enrichment (EnriqRE) factors were estimated in accordance with national environmental regulations. Aluminum (Al) concentrations exceeded the 0.1 mg/L limit in most seasons, indicating ecotoxicological risk and potential bioaccumulation. Iron (Fe) and manganese (Mn) concentrations at some of the analyzed points were below regulatory limits; however, they exhibited accumulation, particularly in treatment tanks (settling basins), followed by release during drier periods.

Overall, the aquaculture facility showed internal accumulation of potentially toxic metals, alternating between retention and release at the discharge and intake points, depending on the season analyzed. The integrated assessment highlights the need for improvements in water management and effluent control in this type of enterprise to ensure the sustainability of regional aquaculture and the protection of aquatic ecosystems.

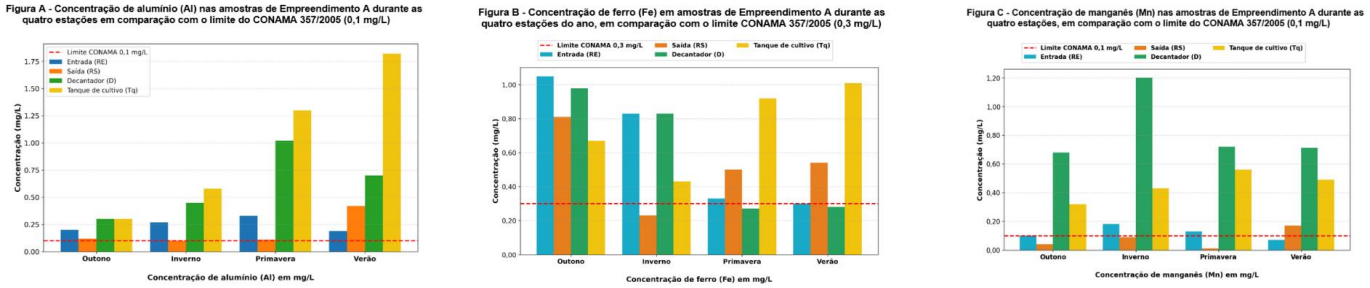


Figure 1: the profile of the seasonal variation in the metals at different points in the fish farm.

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Preparation and physicochemical characterization of eucalyptus-based biosorbents

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Palavras Chave:*Activated carbon,Eucalyptus,Chemical activation,Pyrolysis,Lignocellulosic residues*

Highlights

Eucalyptus wastes were valorized as biosorbents.

Pyrolysis yielded low surface area, similar to in natura biosorbent.

KOH-activated biosorbent reached a high specific surface area of 714.7 m²/g.

Resumo/Abstract

Eucalyptus lignocellulosic wastes are abundant in the Brazilian pulp and paper industry. This study aimed to produce and characterizeeucalyptus-basedmaterials as sustainable biosorbents for wastewater treatment. Firstly, the*in natura*residues (EUC) were dried, ground and sieved. Then, carbonization was conducted under N_2 flow at 350 °C for 120 min to produce pyrolyzed material (PEUC). Finally, chemical activation used KOH with thermal treatment at 750 °C for 90 min in inert atmosphere (AEUC). Biosorbents were characterized by ATR-FTIR, BET, XRD, and pH_pzc. Preparation yields were 34% (PEUC) and 31% (AEUC), relative to EUC. The EUC ATR-FTIR spectrum exhibited characteristic lignocellulosic bands: 3400-3200 cm^{-1} for O-H stretching from cellulose and lignin hydroxyl groups, 2900 cm^{-1} for C-H stretching aliphatic chains, and 1600-1500 cm^{-1} from C=C aromatic rings of lignin. PEUC showed reduced O-H and C-H intensities due to thermal decomposition of cellulose and hemicellulose, while preserving aromatic signal. For AEUC, the band at 1600 cm^{-1} increased and that of O-H decreased, indicating the formation of stable surface carbonaceous groups. Increased basicity raised the pHpzc from 6.9 (EUC) to 7.7 (PEUC/AEUC), favoring anionic adsorption. XRD analysis verified the semi-crystalline structure of EUC (peak at $2\theta \approx 22.5°$), whereas PEUC showed significant intensity reduction and band broadening. Conversely, AEUC presented a predominantly amorphous profile. Surface areas of 0.4 m²/g (EUC) and 1.4 m²/g (PEUC) contrasted sharply with 714.7 m²/g (AEUC) compared to the 595 m²/g area of commercial activated carbon (used as reference), demonstrating the efficacy of chemical activation in increasing surface area. In conclusion, AEUC showed the best potential as a biosorbent. Additional studies are underway for dye and heavy metal removal, enhancing the value of this waste in the circular economy.

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Preparation of Polyvinylpyrrolidone (PVP) Nonwoven Material for Vitamin Release.

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Palavras Chave:*Electrospinning,Anemia,membrane*

Highlights

The parameters studied suggest homogeneous, bead-free fibers. PVP fibers show potential to improve the absorption and bioavailability of the vitamin.

Resumo/Abstract

A vitamina B12 desempenha um papel importante em diversas funções biológicas, destacando-se a formação de glóbulos vermelhos e o funcionamento adequado do sistema neurológico. Apesar da possibilidade de ser obtida pela dieta, estima-se que entre 10% e 15% da população com mais de 60 anos apresenta deficiência dessa vitamina. Nesse contexto, o objetivo desse trabalho é propor uma metodologia de preparo de um não-tecido eletrofiado para liberação rápida da vitamina com a proposta de melhorar a sua absorção e biodisponibilidade. Desse modo, foi preparado uma solução polimérica de PVP a 8% (m/v) solubilizado em uma mistura de etanol:água (80:20) e adicionado a vitamina na proporção de 1% (m/m) em relação a massa do polímero. Com o intuito de melhorar a permeação foi adicionado 0,2% (m/v) de ácido cítrico. A solução ficou sob agitação por 24 horas. Durante a eletrofiação foram realizadas variações de parâmetros, sendo eles: Tensão (10, 12 e 14 quilovolts (kV)), Fluxo de Ejeção (2,8, 3,0 e 3,2 mililitros por hora (ml.h-1) e distância da agulha até o coletor (10 e 12 centímetros (cm)) para posterior avaliação da morfologia por microscopia ótica (MO) e do diâmetro médio das fibras utilizando o software ImageJ. Durante a eletrofiação, a variação de parâmetros permitiu a obtenção de fibras com perfil homogêneo e ausência de Beads para os parâmetros: 12 kV de tensão, 3,0 ml.h-1 de fluxo e 12 cm de distância, apresentando um diâmetro médio de 1856,99±330,49 nanometros (nm). Não obstante, realizou-se um teste de dissolução em meio simulando saliva (pH = 6,8), permitindo observar uma rápida solubilização e estabilidade em 4 minutos. Esses resultados apresentam uma perspectiva positiva para um material que permita uma absorção mais efetiva de Vitamina B12 e, assim, garantindo melhora na qualidade de vida de pacientes acometidos pela deficiência dessa substância.

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Process Development to Increase the Availability of Reactive P for its Recovery from Swine Wastewater

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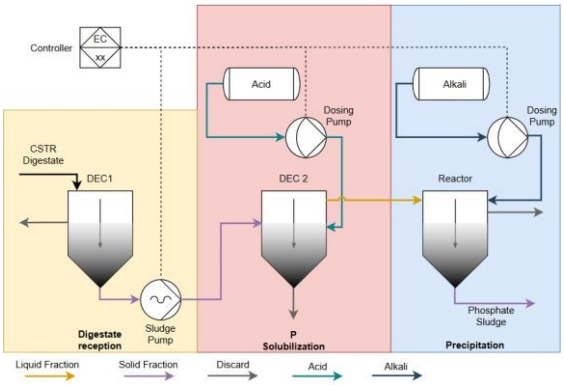
Palavras Chave:*Second Generation P,P fractionation,struvite,fertlizer,digestate*

Highlights

- An automated apparatus was built for P extraction from swine wastewater
- Reactive P availability was increased from 42 to 97%
- Extraction of P using sulfuric acid solution

Resumo/Abstract

Phosphorus is an essential macronutrient for agriculture, however, natural resources are running out and the recovery of P from waste, called second generation P (SGP), has gained attention. In addition, Brazil has to import P to supply its agriculture, which compromises the national sovereignty of the sector. In this sense, Embrapa has been leading some networks to obtain SGP. Swine production wastewater presents P concentrations as a potential source of SGP; however, most of the concentration is not available as PO_4^{3-}(reactive P), avoiding its direct recovery through traditional chemical processes (calcium phosphate or struvite). So, the aim of this work was to develop a process to increase reactive P from swine manure digestate (obtained after anaerobic digestion for biogas production), at laboratory scale. Digestate was sampled from a biodigester installed in a swine wastewater treatment system (Sistrates®, Videira, SC, Brazil). The process of P recovery employed an automated process, shown on Figure 1 and consisted of the following steps: 1) Sedimentation in a decanter (DEC 1); 2) acidification of sludge from step 1 with H_2SO_4 followed by sedimentation of acidified sludge (DEC 2); 3) liquid fraction transference to a reactor for P recovery as an insoluble product: calcium phosphate ($Ca_3(PO_4)_2$) or struvite ($MgNH_4PO_4$). Automation was installed to allow the continuous operation. The volume and concentration of H_2SO_4 to allow safe operation and to get the higher recovery of reactive P considering total P concentration (P_{total}) on digestate were determined, as well as the time required on step 1, 2 and 3, that implies the hydraulic retention time of each step. Without this pretreatment, only 42% was reactive P, while using the optimized conditions and the proposed system, the concentration of reactive P available on step 3 reached 97% of P_{total}, highlighting its applicability to increase the yield of $Ca_3(PO_4)_2$or $MgNH_4PO_4$ production in a next step.



Schematic representation of the apparatus for P extraction and recovery from digestate

Agradecimentos/Acknowledgments

This work was supported by the National Council for Scientific and Technological Development (CNPq) under Grant [number 406144/2022-2].

Remoção de Benzotriazol com as zeólitas ZSM-5 e Ce-ZSM-5

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Palavras Chave:*adsorção,zeólita,troca iônica,meio ambiente,nanoestrutura*

Highlights

Incorporação de Ce em ZSM-5 por troca iônica, sem alteração estrutural. ZSM-5 e Ce-ZSM-5 apresentam adsorção eficiente de benzotriazol em meio aquoso.

Resumo/Abstract

O presente estudo avaliou a eficiência de zeólitas ZSM-5 e Ce-ZSM-5 (incorporada por troca iônica) na remoção de benzotriazol (BTA) em meios aquosos. O BTA é um contaminante emergente utilizado como inibidor de corrosão, frequentemente detectado em corpos d'água. Para sua remoção, os processos de adsorção utilizando zeólitas têm se mostrado alternativas promissoras. A zeólita ZSM-5 tem uma elevada razão Si/Al e caráter hidrofóbico, características favoráveis à adsorção de compostos orgânicos. Modificações superficiais com cério podem aprimorar sua performance adsortiva, uma vez que espécies de Ce são capazes de promover interações de coordenação com o anel triazólico do BTA. Os resultados de difração de raios X (DRX) (Fig. 1) revelaram que todas as amostras apresentam pureza de fase, não sendo identificada a presença de óxido de cério cristalino. Os espectros de ^{29}Si RMN indicaram que a ZSM-5 contém predominantemente sítios Q^4 (4Si,0Al), com sinais em −110 e −112 ppm, refletindo uma maior contribuição de espécies de silício, em concordância com os resultados de XRF. A modificação com cério (Ce-ZSM-5) não promoveu alterações significativas nas posições dos sinais, o que é atribuído à preservação da estrutura cristalina. Os espectros de ^{27}Al RMN de ZSM-5 e Ce-ZSM-5 mostram picos intensos em torno de 60 ppm, indicando a incorporação de alumínio na estrutura zeolítica. O espectro Raman das amostras ZSM-5 e Ce-ZSM-5 mostrou que as vibrações T–O–T da zeólita estão preservadas após a incorporação de Ce. As amostras ZSM-5 e Ce-ZSM-5 demonstraram performances semelhantes na remoção de BTA (≈55%). As isotermas de adsorção apresentaram melhor ajuste para o modelo de Freundlich, indicando superfícies heterogêneas e adsorção multicamada. Por fim, a zeólita ZSM-5 apresenta boa estabilidade operacional por até dois ciclos de reutilização, com retenção da eficiência de remoção.

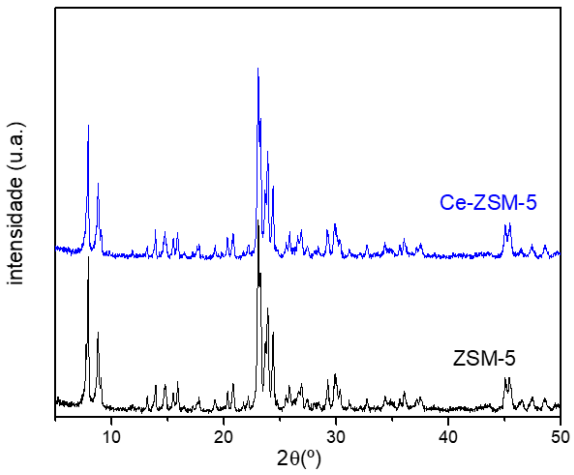


Figura 1 - Difratograma de Raios-X das zeólitas ZSM-5 e Ce-ZSM-5 sintetizadas

Agradecimentos/Acknowledgments

Os autores agradecem à FAPERJ pelo suporte financeiro e à UFES pelas caracterizações das amostras.

Resolvendo dois problemas da indústria de látex natural usando tanino vegetal

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Palavras Chave:*Látex, Hevea Brasiliensis, tanino, alergias, amônia.*

Highlights

Tannin to treat natural latex to avoid the use of ammonia and to eliminate normal allergies to latex articles; Surgeon gloves can be produced without allergies treating the latex with tannin.

Resumo/Abstract

A cadeia produtiva de artigos essenciais como luvas, preservativos, cateteres e balões, produzidos a partir do látex de borracha natural (LBN), enfrenta há décadas dois problemas com consequências para a saúde. O primeiro é o uso de amônia na conservação do látex. Este constitui o citoplasma das células laticíferas da*Hevea brasiliensis*e é vulnerável à rápida degradação biológica e coagulação. A amônia tem servido como biopreservante e estabilizador coloidal para o LBN por mais de 120 anos. No entanto, apresenta sérias desvantagens para a saúde dos trabalhadores: é volátil, irritante, tóxica e cumulativa. Intensas pesquisas por alternativas têm se estendido por mais de 70 anos e, até agora, resultaram apenas na substituição parcial da amônia. Alergias causadas por proteínas do LBN constituem o segundo problema grave na cadeia do látex. A eliminação dessas alergias também tem sido objeto de intensa investigação por mais de 40 anos, e o problema persiste até hoje. Elas variam de simples urticária a casos graves, podendo chegar a choque anafilático e até morte. Pesquisas conduzidas desde 2014 pelo Laboratório TECBOR (IQ/UnB) propõem tanino como base de uma formulação para resolver os dois problemas. Após trabalhos de laboratório, vários experimentos-piloto envolvendo centenas de litros de látex produziram resultados muito promissores. Tais experimentos, livres de amônia, envolveram produção no campo, centrifugação industrial e produção experimental de luvas cirúrgicas. Estas foram testadas e classificadas como não alergênicas em instituto especializado. A base química é a complexação de proteínas do látex pelo tanino, prevenindo o ataque bacteriano e, ao mesmo tempo, inviabilizando reações alergênicas. A mesma abordagem química constitui a base da produção de couro há mil anos. Na sequência dos projetos, está sendo montado um seringal modelo em município perto de Brasília para produção permanente de látex tratado com tanino.



Demonstração das luvas antialérgicas produzidas pelo TECBOR

Agradecimentos/Acknowledgments

FAPDF
TANAC
Fazenda Maíra
IQ/UnB

SÍNTESE DE BIOCARVÃO ATIVADO DE CASCA DE BANANA FUNCIONALIZADO COM Fe_3O_4: CARACTERIZAÇÃO E APLICAÇÃO NA ADSORÇÃO DE AZUL DE METILENO

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Palavras Chave:*Biocarvão,Nanopartículas,Fe_3O_4,Magnetita,Adsorção*

Highlights

Activated biochar from agro-industrial waste was functionalized with Fe_3O_4 magnetic nanoparticles to enhance methylene blue adsorption and enable easy magnetic separation in wastewater treatment.

Resumo/Abstract

O descarte inadequado de efluentes industriais, especialmente provenientes da indústria têxtil, tem contribuído significativamente para a contaminação de corpos hídricos por poluentes emergentes. Dentre esses compostos, o azul de metileno se destaca pela elevada estabilidade química, toxicidade e resistência aos tratamentos convencionais de efluentes. Nesse contexto, a adsorção por biocarvão ativado atua como uma alternativa promissora, devido à sua eficiência, baixo custo e simplicidade operacional.

A síntese de biocarvão ativado a partir de resíduos agrícolas permite uma prática sustentável e capaz de agregar valor ao subproduto agroindustrial, esse reaproveitamento ocorre pela pirólise da biomassa carbonáceo, como as cascas de bananas, promovendo a formação de poros e o aumento da área superficial. Com o objetivo de aumentar o desempenho do biocarvão aplicado no tratamento de efluentes, a técnica de funcionalização da superfície do biocarvão com reagente a base de nitrogênio e ancorar nanopartículas magnéticas de óxido de ferro (Fe_3O_4), possibilita a obtenção de um nanocompósito que responde rapidamente a aplicação de um campo magnético facilitando a separação do adsorvente e o meio aquoso, além de potencializar a área superficial e os sítios ativos do material

Os compostos são caracterizados por técnicas de espectroscopia no infravermelho por transformada de Fourier (FTIR), microscopia eletrônica de varredura (MEV), difração de raios X (DRX), área superficial BET e termogravimetria (TGA). A eficiência adsortiva ainda será avaliada por meio de estudos cinéticos e isotermas de adsorção aplicados à remoção do corante azul de metileno em solução aquosa.

Portanto, a pesquisa propõe um estudo comparativo entre o biocarvão e o biocarvão funcionalizado com Fe_3O_4, avaliando a capacidade de adsorção, facilidade de separação e potencial de reutilização de ambos os materiais, contribuindo para o desenvolvimento de tecnologias sustentáveis no tratamento de efluentes têxteis.



Síntese de biocarvão magnético aplicado na remoção de corantes têxteis

Agradecimentos/Acknowledgments

Agradecimento a infraestrutura do Centro Multiusuário do Centro de Ciências Tecnológicas da Universidade do Estado de Santa Catarina (CMU/CCT/UDESC). Agradecimento aos órgãos CAPES, CNPq, PROMOP e, em especial, a FAPESC por contribuir com a pesquisa.

SYNTHESIS AND CHARACTERIZATION OF CASTOR BEAN HUSK-DERIVED ACTIVATED CARBON BY CHEMICAL ACTIVATION WITH H3PO4

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Palavras Chave:*Activated carbon; biomass; sustainable.*

Highlights

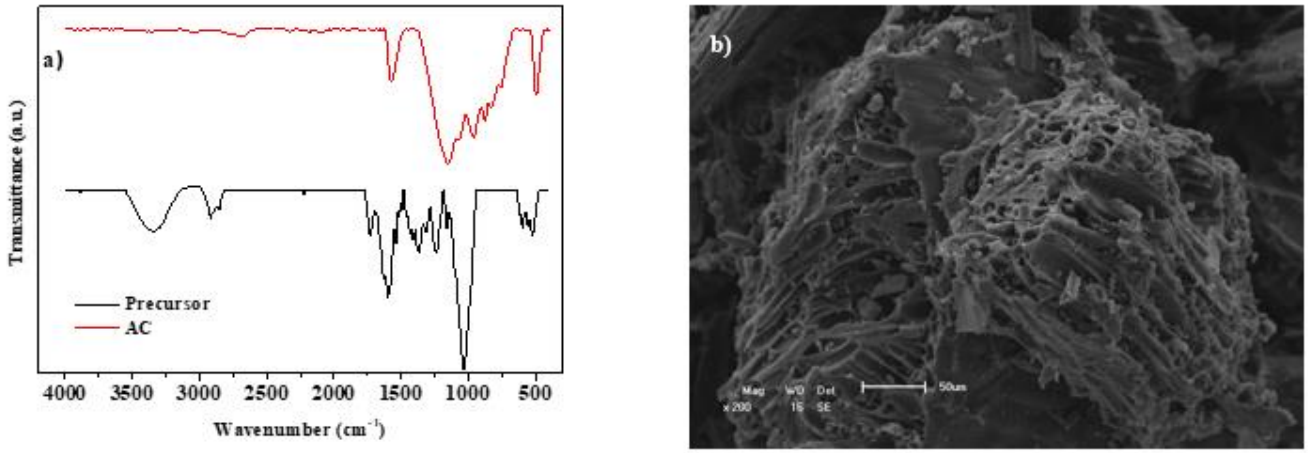
A low-cost and sustainable precursor was used.

Activated carbon was successfully synthesized from castor bean husk.

The activated carbon showed high specific surface area.

Resumo/Abstract

Pollution has become a complex and costly challenge in modern society, as pollutants such as dyes, pharmaceuticals, and industrial chemicals are often recalcitrant to low-cost treatment technologies. Activated carbon (AC) is widely recognized for its high adsorptive capacity and is extensively used in water purification and detoxification. This study aims to synthesize and characterize activated carbon produced from castor bean husk – an underutilized agro-industrial residue – using phosphoric acid (H_3PO_4) as the activating agent. Proximate analysis of the precursor (particle size 250 – 425μm) revealed a moisture content of 8.85%, ash content of 10.11%, volatile matter of 78.04%, and fixed carbon of 11.84%. After activation using the ration 1:1 (precursor-to-H_3PO_4*wt.:v*), a yield of 25.72% was obtained, reinforcing the potential of castor bean husk as a suitable precursor for activated carbon production. Fig. 1a displays the FTIR spectra of the precursor and the AC. The analysis of these spectra allowed for the identification of characteristic functional groups on the material surfaces. The attenuation of the O–H and C–H bands in the precursor spectrum, along with the appearance of P–O–P vibrations in the AC spectrum, evidences the successful activation of the castor bean husk by H_3PO_4. Fig. 1b displays the SEM micrograph of the AC, which exhibits an irregular and heterogeneous structure. This structure results from the H_3PO_4 impregnation followed by slow pyrolysis, yielding an AC with high specific surface area (*SBET*) of 774 m² g–¹. Additionally, the total pore volume was 0.629 cm³ g–¹, with an average pore size of 3.24 nm.



FTIR spectra of the precursor and H_3PO_4-activated carbon and SEM image of the activated carbon.

Agradecimentos/Acknowledgments

The authors acknowledge the State University of Maringá and its analytical center (COMCAP), as well as the funding agencies: CNPq, CAPES, and Fundação Araucária.

Synthesis and Photocatalytic Performance of Pectin/PVA/Corrole Hybrid Films for Degradation Non-Steroidal Anti-Inflammatory Drugs in Aqueous Media

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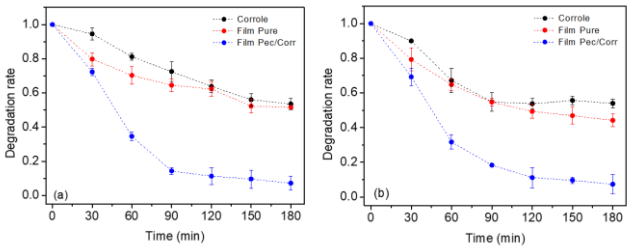
Palavras Chave:*photocatalyst,polysaccharide,corrole,film*

Highlights

Hybrid pectin/corrole films show high photocatalytic activity for NSAID degradation in water. Degradation efficiencies reached 85–97% under visible light. Material is reusable for at least 15 cycles.

Resumo/Abstract

The consumption of pharmaceutical products has increased alongside urbanization, leading to significant contamination of water bodies by pharmaceutical compounds. This contamination poses adverse effects on aquatic ecosystems and human health. Among the primary contributors to this environmental issue are anti-inflammatory drugs. Photocatalytic degradation has emerged as a promising approach, utilizing sunlight or UV light and oxygen to break down pharmaceutical compounds into less harmful products. Due to their photoactive properties, corroles have been extensively studied as photocatalysts. However, in their free form, corroles often suffer from limitations such as low stability in solution and a tendency to aggregate. A common strategy to overcome these drawbacks is the immobilization of corroles onto solid supports. In this work, a photocatalyst based on pectin and 5,10,15-tris(pentafluorophenyl)corrole was developed for the degradation of nonsteroidal anti-inflammatory drugs, with ibuprofen and nimesulide chosen as model contaminants. Thin films were prepared by the*casting*method, wherein the corrole was immobilized within a matrix composed of pectin and polyvinyl alcohol, crosslinked with glutaraldehyde. Comprehensive characterization of the hybrid material was conducted at the University of Coimbra, Portugal, employing scanning electron microscopy (SEM), fluorescence lifetime imaging microscopy (FLIM), as well as absorption and emission spectroscopy. Photocatalytic degradation tests demonstrated that the hybrid films achieved degradation efficiencies ranging from approximately 85% to 97%. The photocatalyst maintained high degradation rates across varying pH values, contaminant concentrations, and catalyst dosages. Additionally, the material exhibited excellent stability and reusability, retaining its photocatalytic performance for at least 15 reuse cycles. Photocatalytic tests under sunlight also confirmed its efficiency, achieving over 80% degradation.



Photocatalytic degradation of (a) ibuprofen and (b) nimesulide solutions 0.1 mM

Agradecimentos/Acknowledgments

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Temporal variability of PM2.5 in São Paulo (2020-2025): implications for pulmonary deposition and respiratory health

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Palavras Chave:*Atmospheric pollution, Particulate matter, Biomass burning, Pulmonary deposition*

Highlights

2024 was the year with the highest concentration of PM2.5

Progressive increase in the number of hospitalizations for respiratory disease

The most deposition of PM2.5 was in upper airway

Resumo/Abstract

Fine particulate matter (PM2.5) air pollution is considered by the World Health Organization (WHO) the fourth leading risk factor for humanity. São Paulo is strongly affected by this pollutant, originating from different sources, including biomass burning, vehicular and industrial emissions. This study evaluated the temporal variation of PM2.5 concentrations in the city of São Paulo between 2020-2025, considering different social-environmental contexts, such as the COVID-19 pandemic and periods of intense wildfires. Sampling was conducted during specific times each year, totaling 218 samples. In 2020 (March to August), a period marked by mobility restrictions, the lowest average in the analyzed interval was observed (17 µg.m-3). Between 2021 and 2024, a progressive increase in mean concentrations was observed (23, 26, 31 and 38 µg.m-3, respectively), with 92% of the samples in 2024 exceeding the WHO recommended daily limit (15 µg.m-3). In 2025, a significant reduction in the mean concentration was observed (19 µg.m-3), coinciding with the lowest wildfire index in Brazil according to INPE. Secondary data from the Brazilian Hospital Information System (DATASUS) indicated a progressive increase in hospitalizations for respiratory disease unrelated to COVID-19 in São Paulo from 2020 to 2023. In addition to the analysis of atmospheric concentrations, pulmonary deposition of PM2.5 was estimated using the Multiple-Path Particle Dosimetry (MPPD) model for adults and children. The simulations indicated a higher fraction and dose of pulmonary deposition in adults more than in children (1.4 to 38.3 µg.h-1 and 1.1 to 29.5 µg.h-1, respectively) with predominance in the upper airway, followed by pulmonary and tracheobronchial region for both groups.. The results indicate chronic population exposure to elevated PM2.5 levels and reinforce the influence of anthropogenic factors and extreme events on urban air quality impacting on human health.

Agradecimentos/Acknowledgments

The authors thank CAPES, CNPq, and FAPESP grants (CAPES PROEX - 88887.175780/2025-00; CNPq; FAPESP 2024/09547-7).

Total Chromium Monitoring in Aqueous Solutions by a Tb(III) Coordination Network:Adsorption Factors, Isotherms, Kinetics, and Structural Stability

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Palavras Chave:*[TbHbtec] n,environmental monitoring,FAAS,negative surface charge,reusability.,Monitoring total Cr species using the [TbHbtec]„ network,Highly durable and reusable for over 100 cycles,The adsorption mechanism elucidated by FIA-FAAS occurs via H- bond-assisted physisorption.*

Highlights

Monitoring total Cr species using the $[TbHbtec]_n$ network. Highly durable and reusable for over 100 cycles. The adsorption mechanism elucidated by FIA-FAAS occurs via H-bond-assisted physisorption.

Resumo/Abstract

Contaminants from heavy-metal ions (HMIs), particularly hexavalent chromium (Cr(VI)), pose serious environmental and human health risks due to their widespread use, discharge into wastewater, and carcinogenic nature [1]. In this work, a Tb(III) coordination network $[TbHbtec]_n$ [2] was investigated as an environmentally friendly and cost-effective nano-adsorbent for monitoring total chromium species in wastewater, synthesized using water as the sole solvent. Its adsorption performance toward chromium species was evaluated [3]. Equilibrium was reached within 15 min, following pseudo-first-order kinetics and physisorption, with adsorption described by Khan and Langmuir isotherms. Zeta potential data indicate that chromium uptake at pH 11 is mainly governed by hydrogen-bond-assisted interactions, despite the negative surface charge of $[TbHbtec]_n$ over pH 3–11. Chromium quantification was performed by flow injection analysis coupled to Flame Atomic Absorption Spectrometry (FIA-FAAS) after adsorption/desorption. The method showed a linear range of 0.1–1.0 mg L^{-1}, limit of detection (LoD) of 0.016 mg L^{-1}, and limit of quantification (LoQ) of 0.052 mg L^{-1},intra- and interday precision ranging from 9.12 to 14.00 % and 0.97–13.91 %, and intra- and interday accuracy ranging from 94.63 to 96.65 % and 85.85–99.04 %. The $[TbHbtec]_n$-packed column exhibited high durability and reusability over more than 100 cycles, confirmed by powder X-ray diffraction. Optimal conditions were pH 11.0, HNO_3 concentration of 0.35 mol L^{-1}, and a preconcentration flow rate of 5.5 mL min^{-1}. Chromium levels in analyzed samples were below regulatory limits.The material retained its crystalline structure after adsorption, demonstrating stability and strong potential for environmental monitoring applications.

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Ubiquity of Microplastics in a Protected Freshwater Ecosystem of the Brazilian Cerrado

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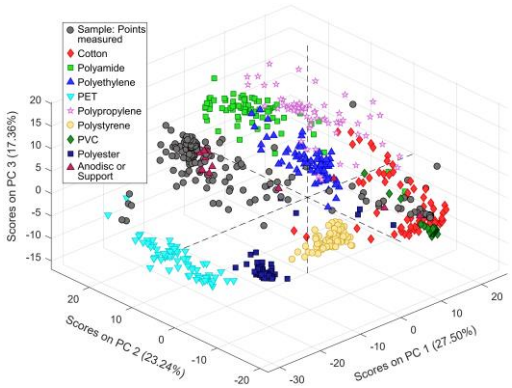
Palavras Chave:*Microplastics,Freshwater,Emerging Contaminants,Micro-FTIR*

Highlights

Microplastics detected in a protected ecosystem of the Brazilian Cerrado. Fiber particles dominance even far from urban centers. Multiple polymers identified by µ-FTIR and chemometrics.

Resumo/Abstract

Freshwater environments can act as sources, transport pathways, and sinks for microplastics, even in preserved ecosystems distant from urban centers. In this context, this study aimed to identify and characterize microplastics in water samples from the Javaes River, located within Araguaia National Park, Tocantins State, Brazil, a protected area of the Cerrado biome. Sampling was performed during two campaigns in the dry (September) and rainy (November) seasons. Approximately 100 L of water were collected at different river sites using 5 L stainless steel bailers and filtered through plankton separation cups (680 µm mesh). The retained material was transferred to 250-mL Schott glass bottles and transported to the Laboratory of Chemometrics and Environmental Chemistry at the University of Brasilia. Samples were filtered using PVDF membranes (47 mm, 0.45 µm), and the retained material was separated by density in JAMSS-type devices using a NaI solution (1.6 g/cm³) for 24 h. The supernatant was subsequently retained on PVDF membranes and analyzed by optical microscopy for shape, size, and color. The material was then transferred to alumina Anodisc membranes (47 mm, 0.2 µm) and characterized by micro-FTIR spectroscopy. Spectra were automatically acquired at 256 points per membrane (16 × 16 grid) and classified using Principal Component Analysis to explore correlations among sampling sites, and Partial Least Squares Discriminant Analysis using normalized reference spectra of common polymers and cotton. Microplastics were detected in both sampling seasons, with a predominance of fibers reaching up to 3.3 mm in length and concentrations ranging from 190 to 427.5 items m^{-3}. The polymers identified included polyamide, polyester, polyvinyl chloride, polypropylene, and polyethylene terephthalate. These results demonstrate the widespread occurrence of microplastics even in protected areas, indicating contributions from distant sources throughout the river basin.



PCA score plot of polymer reference standards and diferent points of a typical sample membrane

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Using proteins from unconventional sources for bioplastics production.

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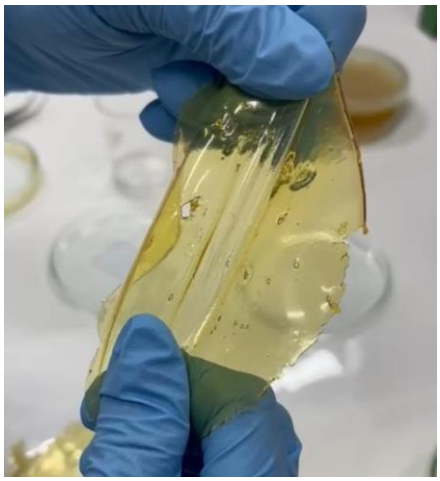
Palavras Chave:*Bioplastic,protein,extraction,characterization,Tenebrio molitor.*

Highlights

Bioplastics for different applications derived from protein from*Tenebrio molitor*larvae.

Resumo/Abstract

The growing search for substitutes for petroleum-derived plastics (polyethylene and polypropylene) has been increasing due to drastic changes in ecosystems caused by pollution (GEYER*et al*., 2017). In this context, bioplastics are an alternative due to their degradability and more sustainable production. There are various methods for obtaining bioplastics, and in this work,*Tenebrio molitor*larvae were used because they are a source of protein, which was one of the components of the target material. The method used to obtain the protein was alkaline hydrolysis (BROGAN*et al*., 2021), a procedure that includes agitation and heating at pH 10.0, followed by centrifugation with acid precipitation at pH 4.5. The isolated protein was then purified through several dialysis steps. For quantification, the Bradford method was used with BSA (Bovine Serum Albumin) as the reference protein (BRADFORD, 1976) and 15% SDS-PAGE acrylamide gel electrophoresis, indicating the presence of proteins but suggesting further purification steps would be necessary. However, these protein samples were used to manufacture bioplastics. Different proportions of extracted protein, glycerol, sorbitol, water, glutaraldehyde, and transglutaminase were used in the bioplastic production process. These changes in proportions drastically affect the final product, allowing for the production of rigid, low-elasticity films, and malleable, highly elastic films. After producing different standard 10mm x 50mm films, standard solubility characterizations, swelling test, bend test, transmittance, and tensile test (ASTM D882) are being performed. Based on water vapor barrier (ASTM E96) and degradability in different real-world and laboratory environments, such as agricultural soil, seawater, and under free atmosphere, the data were analyzed and compared with soy protein, casein, and gluten films (Yi*et al*., 2013; Jafarpour*et al*., 2020).



Elastic bioplastic film made with protein extracted from Tenebrio molitor.

Agradecimentos/Acknowledgments

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Uso de geopolímeros sintetizados com rejeito de mineração na adsorção de Azul de Metileno em solução aquosa.

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Palavras Chave:*Geopolímeros,rejeito de mineração,azul de metileno.*

Highlights

Geopolymers with mining waste for methylene blue adsorption. Utilization of mining waste for the synthesis of different geopolymer materials.

Resumo/Abstract

O Azul de Metileno (AM) é um corante catiônico e possui uma estrutura complexa, dificultando sua decomposição. Seu acúmulo no corpo humano pode desencadear complicações como tumores ou câncer[1]. Assim, uma solução estudada é a utilização de geopolímeros (GP) impregnados com rejeito de mineração (RT) como material adsorvente. Foram sintetizados 4 materiais, sendo o metacaolim (MK) a fonte de aluminossilicato. Para a síntese preparou-se a solução alcalina ativadora com Na_2SiO_3 alcalino e uma solução de NaOH 10 mol/L. Após, adiciona-se 0,1% de H_2O_2, para aumento da porosidade entre 0% e 50% de RT à solução alcalina. Posteriormente, foi adicionado o MK, misturado e aplicado em um molde, onde são submetidos a um tempo de cura de 7 dias em temperatura ambiente. Por fim, foram retirados do molde e colocados em acetona para interromper a cura. Tanto os materiais, quanto o RT foram submetidos a técnicas de caracterizações como espectrofotometria de infravermelho, termogravimetria e difração de raio X. Realizou-se isotermas e testes cinéticos, a fim de analisar a capacidade de adsorção dos materiais. Para a cinética de adsorção do AM, usou-se uma solução de 50mg/L inicialmente, do mesmo. Foram pesados 0,15g de material para 10 ml de solução de corante. O teste variou o tempo de contato de 1 minuto a 48 horas sob agitação de 220 rpm a temperatura de 25°C. Foi realizada a isoterma de cada material variando as concentrações de 20 a 4000 mg/L por 24 horas. As concentrações finais das soluções de AM foram determinadas por UV-vis. O mateiral GP30%R supera o GP0%R após 100 minutos e remove o correspondente a 82% da concentração inicial de AM em 180 minutos (Figura 1). Os resultados dos experimentos foram satisfatórios, demonstrando que os materiais têm boa capacidade adsorvente, além de ajudar a sanar tal problemática.

1. MISRAN, Erni et al. Ultrasonic assisted adsorption of methylene blue using blood clam shell as a low-cost adsorbent. Results in Engineering, v. 23, p. 102715, 2024.

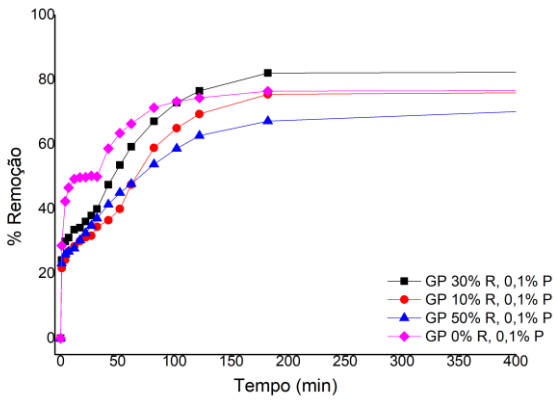


Figura 1: Gráfico cinético AM. R: Rejeito de mineração, P: Peróxido de hidrogênio.

Agradecimentos/Acknowledgments

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Validation and Optimization of Spectrophotometric Methods for the Determination of β-Glucosidase and Arylsulfatase Activities in Soil Samples

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Palavras Chave:*soil,analytical validation,arylsulfatase,β-glucosidase*

Highlights

• Spectrophotometric methods for β-glucosidase and arylsulfatase activity in soils were validated.

• Optimized methods enable reliable and reproducible soil enzymatic activity measurements.

Resumo/Abstract

Soil enzymatic activity is widely recognized as an important indicator of soil quality and health due to its sensitivity to changes in land use and management practices and is commonly associated with enhanced soil organic matter dynamics and carbon sequestration potential. In this context, β-glucosidase (GLI) and arylsulfatase (ARI) are extensively used in agronomic and environmental studies, with their determination traditionally performed by spectrophotometric methods based on*p*-nitrophenol release (Figure 1), as proposed by Tabatabai (1994), using synthetic substrates. Despite their widespread application, to the best of the authors' knowledge, these methods had not been systematically validated according to all analytical figures of merit required by formal analytical chemistry guidelines. Therefore, this study aimed to validate and optimize spectrophotometric methods for determining GLI and ARI activities in soil samples. Matrix effects and key validation parameters were evaluated, including linearity, sensitivity, limits of detection (LOD) and quantification (LOQ), precision, stability, and linear working range. Certified reference materials were not used due to their unavailability for soil enzymatic activity, a limitation still common in this research field. For GLI, matrix effects were assessed by comparing external calibration and the standard addition method. The bilateral Student's*t*-test (95% confidence level) showed no statistically significant difference between the approaches, supporting the use of external calibration. Although a slight tendency toward underestimation was observed, external calibration demonstrated strong correlation with standard addition and superior analytical performance. Both enzymes showed excellent linearity and analytical performance ($R^2 > 0.990$), meeting the criteria established by ANVISA RDC No. 166/2017 and confirming the precision and reliability of the optimized methods.

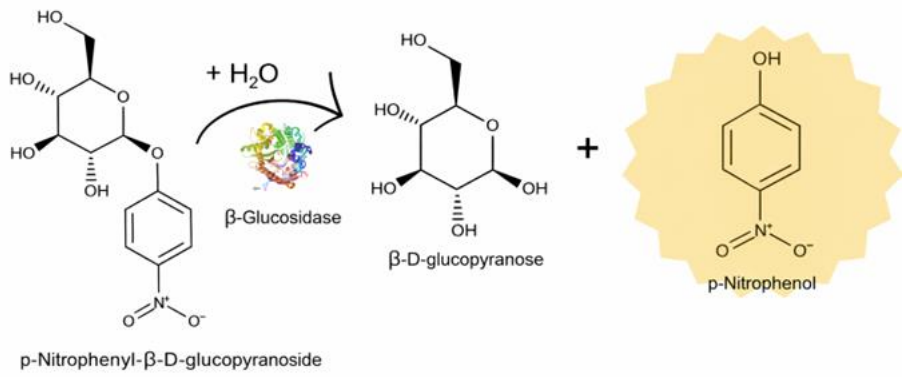


Figure 1: PNG hydrolysis catalyzed by β-glucosidase

Agradecimentos/Acknowledgments

INCTAA – National Institute of Advanced Analytical Sciences

Valorization of hop residue as an adsorbent in the removal of methylene blue dye.

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Palavras Chave:*absorption,Industrial Dyes,coal,Water Treatment.*

Highlights

Sustainable activated carbon was produced from hop extract

The material demonstrated high efficiency in removing methylene blue from aqueous solution

Charcoal made with reused and sustainable extract

Resumo/Abstract

Adsorption is an efficient physicochemical process for removing contaminants from aqueous effluents, using adsorbent materials that retain ionic or molecular species on their surfaces. Despite its wide application, the development of adsorbents with high selectivity, high adsorption capacity, low cost, and sustainable origin remains a challenge. In this context, sustainability is crucial, encompassing raw materials and synthesis processes.

This study proposes the valorization of hop residue—a byproduct of the brewing industry rich in lignocellulose, little explored in the literature compared to residues such as fruit peels or sawdust—for the synthesis of activated carbon, evaluated in the removal of methylene blue (MB) dye from aqueous solutions. Differentiating it from other activated carbons from residues, this material exploits the high natural porosity of hops, chemically activated, promoting greater affinity for cationic dyes. Charcoal was prepared by mixing 5.0 g of hop residue (4.75 µm) with 20 mL of 0.1 mol L^{-1} NaOH, followed by heat treatment at 200 °C for 24 h. Performance was investigated through kinetic and isothermal studies.

The kinetics followed a pseudo-first-order model (R^2 = 0.9957), with q_e = 8.450 ± 0.090 mg g^{-1} and k_1 = 0.113 ± 0.004 min^{-1}, indicating rapid adsorption by physicochemical forces. Isotherms with initial MB concentrations from 0.5 to 100 mg L^{-1} (0.5 mg adsorbent, 5.0 mL solution) revealed favorable behavior.

Activated carbon from hop residue stands out for its efficiency at low dye concentrations, with real potential for treating textile effluents on a pilot scale, combining sustainability and reduced cost.

Agradecimentos/Acknowledgments

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What do caffeine reveal about urban pressure in the Atibaia River? Evidence from a multivariate analysis.

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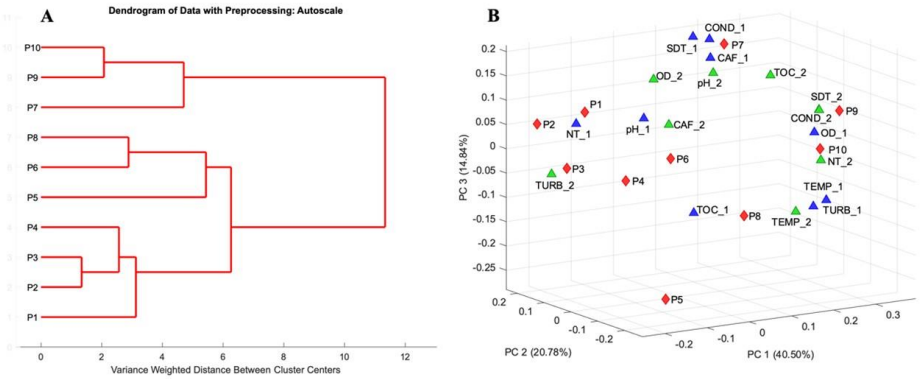
Palavras Chave:*Caffeine, Urban sewage, Surface waters, Physicochemical parameters, Multivariate analysis*

Highlights

Hydrological conditions controlled spatial patterns. Multivariate analysis revealed urban pressure gradients. Sewage inputs were enhanced during peak flow events.

Resumo/Abstract

Caffeine (CAF) is one of the most consumed and frequently detected pharmaceutically active compounds in aquatic environments, being widely used as a tracer of untreated domestic wastewater. This study evaluates the relationship between physicochemical parameters and the concentrations of CAF at different sites along the Atibaia River (Campinas, SP, Brazil). Surface water samples were collected at ten sites during the rainy and dry seasons, in areas influenced by agricultural, residential, and/or industrial activities. CAF was quantified after solid-phase extraction by liquid chromatography–tandem mass spectrometry. Multivariate statistical analyses, including Principal Component Analysis (PCA) and cluster analysis applied to autoscaled data, were used to assess spatial and seasonal patterns. The results revealed strong seasonality between high- and low-flow conditions, with total nitrogen, turbidity, dissolved oxygen, total dissolved solids, total organic carbon, conductivity, and CAF showing marked separation between periods, indicating a strong dependence on hydrological conditions. In contrast, pH and temperature exhibited low seasonal variability. Site P7, located downstream of the Anhumas stream, stood out due to its isolation in the dendrogram and elevated CAF concentrations during high-flow conditions, suggesting increased loads associated with recent domestic wastewater inputs and urban overflows. High CAF levels were also observed at site P2, downstream of the Pinheiros stream, and at sites P9 and P10, corresponding to the main mixing zone between the Atibaia River and the Anhumas stream, while the remaining sites showed intermediate conditions. These findings reinforce CAF as an effective tracer of urban sewage and demonstrate the importance of integrating chemical markers, multivariate analysis, and seasonal variability to assess anthropogenic pressures, highlighting the role of tributary inputs in controlling CAF distribution along the Atibaia River.



Multivariate analysis highlights seasonal effects and CAF enrichment at sites P7, P9–P10, and P2.

Agradecimentos/Acknowledgments

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49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

ANA - Química Analítica

Accurate determination of alkaline and alkaline-earth elements in crude oil by MIP OES after microwave-assisted extraction

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Palavras Chave:*Sample preparation,Crude oil,Alkaline and alkaline-earth elements,MIP OES,Green chemistry*

Highlights

High sample mass using MAE (10 g) enabled very low quantification limits for alkaline and alkaline-earth elements. The method allows simultaneous determination of Ba, Ca, K, Mg, Na, and Sr by MIP OES.

Resumo/Abstract

The presence of alkaline and alkaline-earth elements in crude oil may cause corrosion and salt deposits on the distillation columns and piping. Therefore, precise methods for quality control of these elements are necessary. However, projection and limited sample mass are typical problems when closed systems and concentrated acids are used for digesting this type of matrix. To overcome these problems, extraction with diluted solutions, or even water, can be used. When combined with the use of auxiliary energy sources, such as microwaves, this approach presents a promising alternative. In the present work, the microwave-assisted extraction (MAE) method was developed for further Ba, Ca, K, Mg, Na, and Sr determination in crude oil by microwave-induced plasma optical emission spectrometry (MIP OES). To assess the analytical, environmental, and practical requirements of the MAE method, the White Analytical Chemistry (WAC) metric was employed. The following experimental parameters were evaluated: sample mass, extraction solution volume (H_2O), time, and temperature. Under optimized conditions (10 g, 15 mL, 20 min, and 240 ºC), no statistical difference (t-test, confidence level 95%) between the results obtained by MAE method and the reference values (digestion method) were observed. Due to the use of a high sample mass (10 g), the quantification limits were very low (ranging from 0.001 to 0.1 µg g^{-1}, for Ba and Na, respectively). The proposed MAE method can be considered a simple and fast tool for sample preparation of crude oil for further Ba, Ca, K, Mg, Na, and Sr determination at low concentrations. Furthermore, the determination by MAE and MIP OES proved to be a good option for the simultaneous determination of these elements in crude oil, obtaining higher scores in analytical, environmental, and practical criteria. In this way, the MAE method can be used as an accurate alternative method for routine analysis in the petroleum industry.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPERGS, and PRH 52.1

A CHIRAL LC-MS APPROACH REVEALS CARBOXYLESTERASE-MEDIATED ENANTIOSELECTIVE METABOLISM OF THE ORGANOPHOSPHATE PESTICIDE MALATHION AND MALAOXON

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Palavras Chave:*Chiral LC-MS,microsomes,enantioselectivity,organophosphate,Microsomes*

Highlights

1) CHIRALPAK® IK-3 enabled optimal enantioresolution; 2) Human recombinant CES1 metabolized (R)-enantiomers up to 12× faster than (S)-forms; 3) Enzyme knowledge supports risk assessment

Resumo/Abstract

Malathion is a widely used pesticide with stereochemistry-dependent disposition. Its oxidation product, malaoxon, displays greater insecticidal activity. Enantioselective effects are known in several organisms, but their implications for humans remain unclear. To address this need, this work describes the development of an enantioselective analytical method. A comprehensive screening of seven polysaccharide-based chiral stationary phases was performed under multimodal elution (normal-phase: hexane/alcohol; reversed-phase: water/organic; and polar organic mode: 100% organic). Simultaneous baseline resolution for all enantiomers was achieved within a single run only using the CHIRALPAK® IK-3 column using water:methanol:acetonitrile (35:60:5) as mobile-phase, providing the balance between selectivity and run time. Sample preparation via dispersive liquid-liquid microextraction (DLLME) was developed using one-factor-at-a-time and definitive screening design approaches. The optimal protocol used 540 µL of dichloromethane:methanol (70:30) for 200-µL samples, with agitation (1500 rpm, 2 min) and centrifugation (10000 ×g, 2 min, 4 °C) before evaporation and reconstitution. The method was validated following ICH M10 guideline, showing linearity, precision, and accuracy for enantiomer quantification. As a result, the method was applied to*in vitro*incubations with human liver microsomes and recombinant hCES1 and hCES2 enzymes. Results revealed a pronounced metabolic enantioselectivity: (*R*)-malathion and (*R*)-malaoxon were metabolized by hCES1 approximately 1.7 and 12-fold faster than their (*S*)-enantiomers, respectively, while hCES2 showed no contribution.*In vitro–in vivo*extrapolations indicated limited systemic persistence but significant metabolite formation that may influence toxicological outcomes. This study highlights that chiral separations and miniaturized extraction techniques are essential for the accurate toxicological risk evaluation of chiral pesticides.

Agradecimentos/Acknowledgments

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Alternative chemical analysis: From building to fundamentals in many analytical chemistry techniques

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Palavras Chave:*analytical chemistry, analysis, arduino, do it yourself*

Highlights

- Low-cost equipments in chemical analysis;
- UV-Radiometer and spectrophotometer build up using arduino free-hardware;
- Chemistry principles in Analytical Chemistry.

Resumo/Abstract

Chemical analysis is a fundamental field in chemistry as a whole. Chemical reactions are analyzed usually withdrawing samples at regular time intervals in order to ascertain the chemical changes and reaction behavior. However, some reaction can occurs so fast that the reaction handling and analysis can not be carried out using this approach. In this way, many efforts have been devoted in developing sensors to measure the chemical reactions in situ in real time with reliable results, consistency and reprodutibility. Such premisses are aligned to the 11th principle in Green Chemistry Guidelines. This work show the development of 2 prototypes using the free-harware arduino and correlated hardware boards (e.g. ESP32), they are: i) a UV-sensor working as a UV-radiometer into 290-380 nm and; ii) a spectrophotometer based on a image sensor using RGB parameters. All the prototypes were built according the needed, that is, the time interval of analysis can be described in the prompt command using IA as an important tool in refining the programation language. Figure 1 show A) the measurement of a metallic vapor lamp radiation compared to the sunlight using the UV-sensor and B) spectra of Rhodamine B using the RGB based spectrophometer developed in this work. Adjustments are in course in order to improve the analysis using a flow-system.

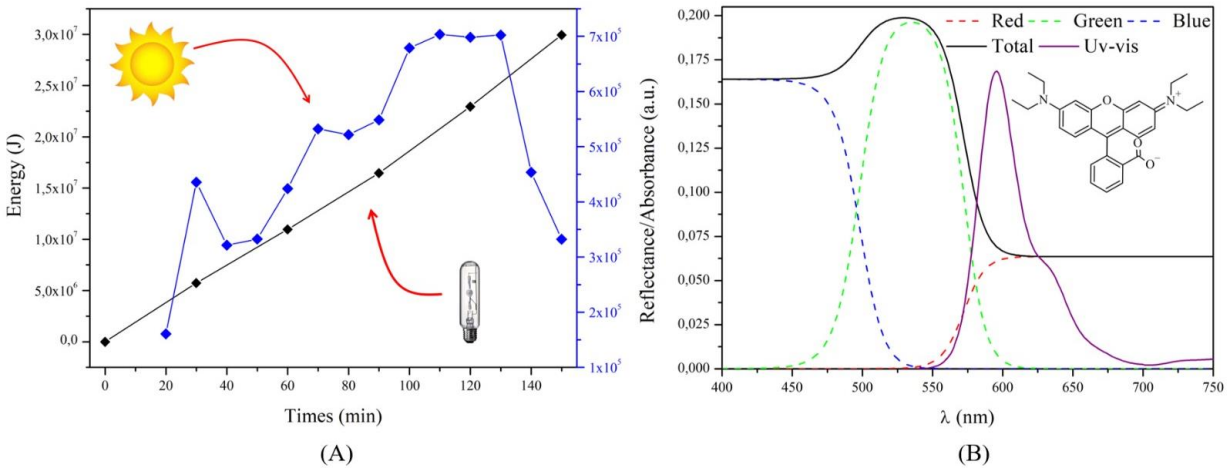


Figure 1. A) Radiometer measurement (lamp x sunlight) and B) RGB measure from Rhodamine B

Agradecimentos/Acknowledgments

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Análise direta de elementos químicos em água do mar por ICP-MS acoplado com sistema High Matrix Introduction (HMI)

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Palavras Chave:*ICP-MS,HMI,água do mar,elementos-traço,matriz salina*

Highlights

•Direct seawater analysis by ICP-MS without pretreatment
•High Matrix Introduction improves plasma robustness in saline matrices
•Low quantification limits and high accuracy achieved in complex samples

Resumo/Abstract

A análise da água do mar por ICP-MS apresenta limitações pela elevada salinidade da matriz, que pode causar supressão de ionização, interferências poliatômicas e instabilidade instrumental. Geralmente, esses efeitos são minimizados por diluições elevadas ou remoção da matriz, aumentando o tempo analítico e o risco de contaminação. Neste trabalho, avaliou-se o desempenho do ICP-MS equipado com o sistema HMI para a determinação direta de elementos dissolvidos, com ênfase na otimização de parâmetros instrumentais e robustez do método.

As amostras analisadas corresponderam à fração dissolvida da água do mar, obtida após filtração em membranas de 0,45 µm e acidificação. As determinações foram realizadas diretamente no ICP-MS, sem pré-tratamento adicional. O instrumento operou em modo HMI, com potência de RF de 1600 W, profundidade de amostragem de 10 mm, gás de nebulização de 0,65 L min^{-1} e diluição do aerossol com argônio (0,26 L min^{-1}), assegurando maior robustez do plasma. A remoção de interferências espectrais foi realizada em célula de colisão operando em modo He (4,5 mL min^{-1}). As curvas analíticas foram preparadas em matriz salina de NaCl 3,5% (m/v), visando compatibilidade de matriz entre padrões e amostras. Os cones de interface foram previamente condicionados com amostra real de água do mar, visando estabilizar a resposta instrumental devido à deposição de sais na interface. Foram monitorados os isótopos ^{27}Al, ^{75}As, ^{114}Cd, ^{59}Co, ^{52}Cr, ^{63}Cu, ^{56}Fe, ^{55}Mn, ^{58}Ni, ^{206}Pb, ^{120}Sn, ^{51}V e ^{66}Zn.

Os limites de quantificação variaram entre 0,027 e 4,23 µg L^{-1}. A exatidão foi avaliada por meio da análise dos materiais de referência certificados ERM-CA403 e CASS-6, com recuperações entre 90% e 108%. Os resultados demonstram que a combinação do HMI, curvas em matriz compatível, pré-condicionamento dos cones e célula de colisão em modo He permite a análise direta de matrizes altamente salinas, com elevada precisão, sensibilidade e estabilidade instrumental.

Agradecimentos/Acknowledgments

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Analysis of tartrazine yellow in isotonic beverages using multiple injection in capillary electrophoresis

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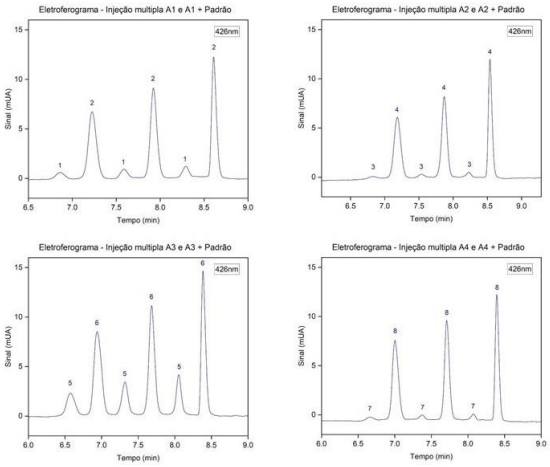
Palavras Chave:*Capillary electrophoresis,Tartrazine yellow,multiple injection,isotonic beverages*

Highlights

MEKC-UV method for tartrazine in isotonic beverages; efficient separation from Sunset Yellow. Multiple injection with single-point standard addition. Good precision (RSD 1,09%) and accuracy (92,7%)

Resumo/Abstract

The synthetic dye tartrazine yellow (E102), widely used in isotonic beverages, has been the subject of discussions regarding its toxicological safety, highlighting the need for reliable analytical methods for its monitoring. In this study, a method for the determination of tartrazine yellow in isotonic beverages was developed and evaluated using micellar electrokinetic chromatography (MEKC) with direct UV–Vis detection. The proposed method enabled the efficient separation of tartrazine from other dyes commonly present in commercial formulations, such as Sunset Yellow FCF (E110), avoiding signal overlap. The methodology employed a multiple-injection strategy combined with single-point standard addition, allowing the sequential analysis of sample, spiked sample, and standard within a single electrophoretic run, thereby increasing analytical throughput and reducing reagent consumption. The running electrolyte consisted of a sodium tetraborate buffer containing sodium dodecyl sulfate (SDS). The analytical performance of the method was assessed through precision (RSD = 1,09%), accuracy (92,7%), limit of detection (0,53 mg L^{-1}), and limit of quantification tests (1,75 mg L^{-1}), using six authentic replicates. The method was applied to the analysis of four isotonic beverages commercially available in the Brazilian market, demonstrating its suitability for quality control analyses and presenting advantages in terms of analytical sustainability when compared to conventional chromatographic methods.



Electropherograms of multiple injections of samples in triplicate.

Agradecimentos/Acknowledgments

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Analytical Characterization of Exosomes from Breast Milk using Different Isolation Methods: Ultracentrifugation and Size-Exclusion Chromatography

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Palavras Chave:*Exosomes,Breast milk,Analytical Characterization,Ultracentrifugation,SEC-HPLC*

Highlights

Comparison of Different Isolation Methods of Breast Milk Exosomes
Ultracentrifugation and Size-Exclusion Chromatography were compared
Analytical characterization was performed and SEC-HPLC was chosen

Resumo/Abstract

Exosomes are nanosized extracellular vesicles (30–150 nm) secreted by most cell types and found in fluids such as blood, urine, and human breast milk. They carry proteins, lipids, and nucleic acids that mediate intercellular communication and regulate physiological and pathological processes. Owing to their biocompatibility, stability in circulation, and natural cargo delivery capacity, exosomes are being explored as disease biomarkers and nanocarriers for targeted therapies, with applications in cancer treatment, tissue regeneration, and immunomodulation. Nevertheless, the absence of standardized, reproducible isolation and characterization methods still limits their clinical translation. Human breast milk is an accessible and biologically relevant source of exosomes, characterized by low immunogenicity and cross-species tolerance that enhance therapeutic potential. However, isolating these vesicles is challenging due to abundant contaminants such as fat globules and casein micelles, which can co-isolate and reduce sample purity. Consequently, optimized isolation and purification strategies are required to obtain high-quality exosome preparations suitable for downstream analyses and biomedical applications. Currently, several isolation techniques are employed, including ultracentrifugation, membrane ultrafiltration, density gradient centrifugation, polymer-based precipitation, size-exclusion chromatography, immunoaffinity capture, and microfluidic approaches, each with specific advantages and drawbacks. In this study, exosomes from donated human breast milk samples obtained from the Milk Bank of the Central University Hospital of Asturias (HUCA) were isolated using ultracentrifugation and size-exclusion chromatography. The isolated vesicles were characterized by total protein quantification (BCA assay), SEC-HPLC, TEM and flow cytometry to evaluate and compare the performance of both isolation methods.

Agradecimentos/Acknowledgments

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Analytical Evaluation of NADES-GFAAS Compatibility for Potentially Toxic Element Determination

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Palavras Chave:*NADES,GFAAS,interferences,sample preparation*

Highlights

Analytical evaluation reveal high compatiblity of NADES-GFAAS and synergistic effects with chemical modifier. The NADES–GFAAS approach shows great potential for the determination of toxic elements.

Resumo/Abstract

Deep eutectic solvents (DES) have been extensively studied in recent years, as evidenced by the large number of publications across various fields of Chemistry. Natural deep eutectic solvents (NADES), a subclass of DES, are composed of natural precursors such as organic acids, amino acids, sugars, and alcohols. They have attracted considerable attention due to their alignment with Green Chemistry principles and their versatility, particularly in sample preparation. In this study, NADES based on citric acid (Ac), lactic acid (Al), choline chloride (ClCo), and glucose (Gli) were evaluated as extraction solvents in sample preparation for the determination of As, Cd, and Pb—elements whose toxicity in humans is well established. NADES prepared at a molar ratio (mol) of 1:1:10 (component 1: component 2: water) resulted in a colorless, homogeneous solution free of precipitates, which are desirable characteristics for extractants/solvents used in sample preparation. Two distinct sample preparation strategies were employed (vortex agitation and ultrasound-assisted), and the compatibility of NADES with graphite furnace atomic absorption spectrometry (GFAAS), was also evaluated. This study was carried out by assessing spectral and/or non-spectral interferences arising from the applied reactional and instrumental conditions, using chemometric tools such as experimental design. The combined evaluation of the parameters: recovery (%), signal-to-background ratio (SBR), and characteristic mass (m_0) was essential for assessing spectral and/or non-spectral interferences in the analyte signals in GFAAS. In addition to the ability of NADES to extract the studied analytes using the simplest method (vortex agitation at room temperature), a potential synergistic effect between NADES constituents and chemical modifiers for the analytes As, Cd, and Pb in GFAAS was observed. This makes the application of NADES highly promising for Analytical Chemistry.

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Application of Er and Nd MOFs in the adsorption removal of Ciprofloxacin from water.

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Palavras Chave:*MOFs,Microwave synthesis,Emerging contaminants.*

Highlights

Microwave energy;

Emerging contaminants;

Strategic elements;

Metalorganic structures;

Resumo/Abstract

Some widely used drugs, such as ciprofloxacin, are not fully metabolized and end up contaminating water bodies. Due to bioconcentration, it remains in this environment even after conventional water treatment, requiring techniques to remedy this need. Thus, this study aims to investigate the adsorption of ciprofloxacin (CPX) in aqueous media using metal-organic frameworks (MOFs) obtained by microwave-assisted solvothermal (MW) method. The MOFs were synthesized in a Mars6 MW reactor for Er3+ (Er-MOF) and Nd3+ (Nd-MOF) MOFs. In the reaction, 0.5 mmol of the precursor salt of each rare earth ion was added to 1.0 mmol of terephthalic acid (H2BDC) and 10 mL of DMF under ultrasonic bath for 20 minutes. The mixture was transferred to PFA tubes and subjected to MW with a 5 min ramp (700 W), followed by a 236 min dwell (250 W) at 160 °C. The MOFs obtained were characterized by SEM-FEG and BET surface area analysis, where rod-like morphologies with an area of 1.96 m^2/g for Er-MOF and irregular agglomerates with 2.82 m^2/g for Nd-MOF were obtained, areas considerably smaller than those reported in the literature, due to the use of MW as an alternative for synthesis. CPX quantification in the adsorption tests was performed by HPLC, phase A: 0.001% formic acid and B: ACN, gradient, in C18 25 cm with wavelengths of 278, using the following calibration curve (y = 168.36692x -51.13026), with R^2=0.999 and LOD/LOQ (mg L^{-1}) of 0.188/0.626. Preliminary adsorption tests were performed at 25°C with 10 mg of each MOF in 50 mL of 10 mg L-1 CPX solution, with magnetic stirring at 400 rpm, with sampling points between 30 and 300 seconds. The results, although preliminary, showed CPX adsorption of 13% in Er-MOF and 19% in Nd-MOF, indicating that the materials obtained by MW are promising for CPX adsorption in environmental samples.

Agradecimentos/Acknowledgments

The authors would like to express their gratitude to FAPEMIG, CNPq, CAPES, and FINEP for their financial support. We thank the Microscopy Center of the Federal University of Alfenas for their technical support and for conducting the experiments.

Application of XRD and SEM–EDS in the Forensic Investigation of Wet Damage in Containerized Cargo during Maritime

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Palavras Chave:*SEM-EDS,X-ray Diffraction (XRD),Maritime Transport,Cargo Wetting and Containers*

Highlights

Forensic SEM-EDS/XRD analysis and chloride quantification of dry cargo wetting;

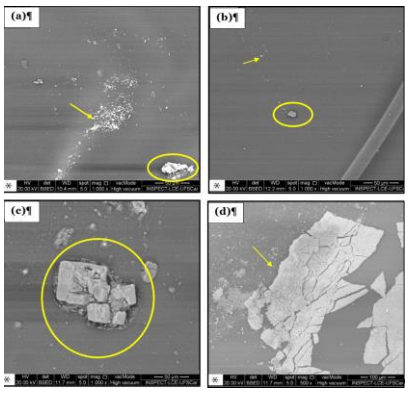
Halite (NaCl) as a definitive seawater marker;

Robust source identification for maritime civil liability.

Resumo/Abstract

Wet damage in containerized cargo represents a challenge in forensic investigations, particularly when distinguishing freshwater from seawater exposure. This distinction is essential for establishing civil liability in delayed investigations, when inspections occur long after the event and the cargo has dried. In this study, an integrated analytical approach was used to characterize mineral residues on cardboard and plastic packaging materials from a maritime container transport case. Field samples (one wet cardboard fragment, two plastic fragments, and residual water) were compared with six laboratory reference samples (three cardboard and three plastic fragments) prepared under three conditions: dry, freshwater-wetted, and seawater-immersed. Samples were analyzed by chloride quantification, scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), and X-ray diffraction (XRD). SEM-EDS analyses were performed using a FEI Inspect S50 microscope with oven-dried, gold-coated samples. Mineral phases were identified by XRD using a Bruker D8 Advance ECO diffractometer (Cu Kalpha1 radiation, 40 kV, 25 mA), scanning from 5 to 90 deg (2theta) at 5 min-1. The investigated water sample showed low chloride concentration (20 mg/L). Packaging materials also exhibited low sodium content and no crystalline halite (NaCl), detected only in seawater reference samples. These results indicate freshwater as the source of the damage and demonstrate the forensic applicability of the proposed methodology.

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SEM micrographs of plastic (1000×): (a) dry, (b) freshwater, (c) seawater, (d) investigated sample.

Agradecimentos/Acknowledgments

The authors thank Critério Experts for providing loss investigation experience and authorizing the use of non-confidential data, and André Lopes for his assistance in text revision.

Artificial Neural Network Model for Tuberculosis Outcome Classification Using Brazilian Public Health Data

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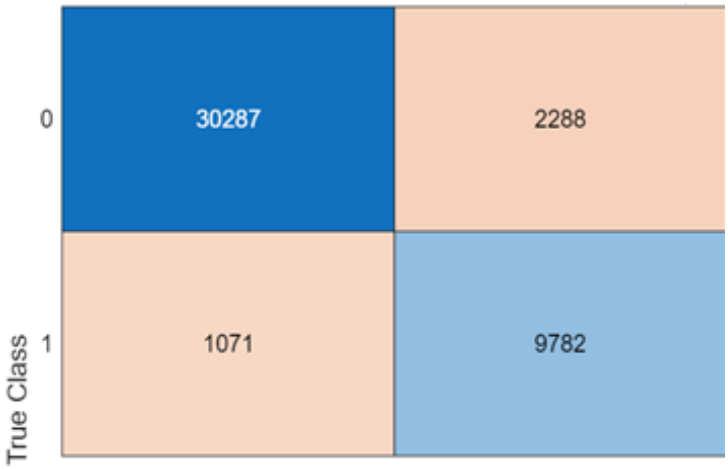
Palavras Chave:*Artificial Intelligence; Neural Networks; Tuberculosis; Public Health Data; Chemometrics*

Highlights

1. Neural network model for TB outcome prediction using SINAN data.
2. High sensitivity supports epidemiological screening.
3. AI applied to large-scale public health datasets.

Resumo/Abstract

Tuberculosis (TB) remains a major public health challenge, with treatment abandonment and mortality contributing to persistent transmission and healthcare burden. This work presents the development of an Artificial Intelligence model based on a Multi-Layer Perceptron Artificial Neural Network (ANN) to classify TB case outcomes using national epidemiological data from the Brazilian SINAN database. The original dataset comprised 964,099 records and 97 variables. Data preprocessing included removal of non-predictive attributes, mean imputation of missing numerical values, min–max normalization, and class balancing by downsampling, resulting in 144,760 samples in an approximate 3:1 ratio between negative and positive classes. The ANN was implemented in MATLAB®, using two hidden layers (40 and 20 neurons), backpropagation training, regularization parameter of 0.15, and a 70/30 training–test split. Output probabilities were converted to binary classes using a decision threshold of 0.210 to prioritize sensitivity. In the independent test set, the model achieved 92.42% accuracy, 80.82% precision, 90.71% sensitivity, and an F1-score of 85.48%. The high sensitivity indicates strong capability to identify cases associated with the outcome of interest, which is critical in epidemiological screening scenarios where false negatives must be minimized. The results demonstrate that ANN-based predictive modeling can function as a chemometric data analysis tool applied to public health, supporting early identification of high-risk TB cases and contributing to optimized resource allocation and surveillance strategies. This approach highlights the potential of analytical data science methods to enhance decision-making in large-scale health information systems.



Matriz de confusão do modelo de Rede Neural Artificial

ASSESSING THE IN VITRO INHIBITION POTENTIAL OF KEY HUMAN CYP450 ENZYMES BY THE HERBICIDE GLYPHOSATE AND ITS MAIN METABOLITE, AMPA

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Palavras Chave:*pesticide, glyphosate, AMPA, in vitro inhibition, human liver microsomes*

Highlights

The inhibitory potential of glyphosate's primary metabolite, AMPA, was investigated.

CYP3A4/5 and CYP2C9 enzymatic activities were affected by glyphosate exposure.

Resumo/Abstract

Glyphosate (GLYP) is the most extensively used herbicide worldwide. Growing evidence indicates the widespread occurrence of GLYP and its main metabolite, aminomethylphosphonic acid (AMPA), in surface and groundwater, atmospheric air, and food products, raising concerns regarding human exposure. If absorbed, these compounds may interfere with xenobiotic metabolism by inhibiting cytochrome P450 (CYP450) enzymes or acting as their substrates, potentially leading to pesticide–drug interactions. In this context, the present study aimed to evaluate the*in vitro*inhibitory potential of GLYP and AMPA on major CYP450 isoforms involved in human metabolism by using human liver microsomes (HLM). An LC–MS method was developed for the determination of probe substrate, internal standard, and metabolite biomarker for each CYP enzyme. Chromatographic separation was performed on a Waters XBridge BEH C18 column (100 × 4.6 mm, 3.5 µm). The mobile phase was delivered at 0.5 mL min^{-1} under gradient conditions, employing water and methanol containing either 0.1% (v/v) acetic acid or 0.05% (v/v) ammonium hydroxide, depending on the ionization mode. MS parameters, including*m/z*values as well as capillary and cone voltages, were optimized individually for each analyte. Sample preparation involved liquid–liquid extraction with ethyl acetate. After mixing and centrifugation, the organic layer was collected, dried under vacuum, and reconstituted in the mobile phase. Initial inhibition screening revealed a statistically significant reduction in CYP3A4/5 and CYP2C9 activities compared with the negative control (t-test, $\alpha = 0.05$) in the presence of 100 µmol L^{-1} GLYP, whereas no significant effect was observed for AMPA at the same concentration. Subsequently, IC_{50} values were determined after 5 and 30 min of preincubation with GLYP. For CYP3A4/5, IC_{50} values were 18 ± 5 mmol L^{-1} and 20 ± 5 mmol L^{-1}, respectively, while for CYP2C9 they were 13 ± 9 mmol L^{-1} and 11 ± 5 mmol L^{-1}, respectively.

Agradecimentos/Acknowledgments

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Assessment of fipronil residues and its degradation products in sugarcane by GC-MS

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Palavras Chave:*Pesticides,Fipronil residues,Degradation products,Sugarcane,Food Safety*

Highlights

A fast and reliable QuEChERS–GC-MS method was developed to monitor fipronil and its toxic degradation products in sugarcane and sugarcane juice, supporting food safety.

Resumo/Abstract

Fipronil is a phenylpyrazole insecticide widely used in sugarcane cultivation due to its high effectiveness against soil pests such as Sphenophorus levis. However, its persistence in the environment and formation of toxic degradation products, including fipronil sulfide, fipronil sulfone, and fipronil desulfinyl, have raised concern, as these compounds may be as toxic or more than the parent molecule. Sugarcane (Saccharum officinarum L.) is one of Brazil's most important crops, with São Paulo state accounting for over half of national production. This study aims to develop, optimize, and apply an analytical method based on QuEChERS extraction coupled with gas chromatography-mass spectrometry (GC-MS) for simultaneous determination of fipronil and its main degradation products in sugarcane and sugarcane juice. GC-MS analysis used internal standard calibration with isotopically labeled fipronil-^{13}C. The method enabled analysis of all compounds within 8 minutes, using splitless injection and selective ion monitoring (SIM). Thirty samples of raw sugarcane and juice were collected from major producing regions in São Paulo, including Ribeirão Preto, Limeira, and Leme. Sample preparation followed a QuEChERS-based protocol using acetonitrile, $MgSO_4$, CH_3COONa, and dispersive SPE sorbents (PSA and C18). The method will be evaluated for chromatographic performance, extraction efficiency, matrix effects, recovery, precision, accuracy, and sensitivity. Results are still being acquired and processed, so conclusive data cannot yet be presented. These ongoing experiments will support the future application of the method for determining fipronil residues and its degradation products in sugarcane and sugarcane juice.

Agradecimentos/Acknowledgments

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AutoDrop – An Automated IoT-Controlled Titrator based on Drop Counting

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Palavras Chave:*Redox Titration,Acid-Base Titration,RS-232,ESP32*

Highlights

Titrator based on countig-drop for instrumental titration
Wi-Fi communication for controling and receive data by realtime and titration

Resumo/Abstract

In this work, we present a significant improvement to drop-counting titration [1]. Drop detection, previously a bottleneck, was redesigned using a modulated IR signal through a narrow channel. This setup blocks stray ambient light and allows for the measurement of the drop's transit time. Simple, low-cost micro-solenoids are used instead of expensive analytical-grade instruments. By controlling the diameter and surface of the capillary, it is possible to obtain drop volumes ranging from 1µL up to 50 µL or higher. A Mariotte bottle was used as the titrant reservoir to stabilize the repeatability of the drop volume. An ESP32 microcontroller receives the serial signal, and various commercial or homemade instruments (RS232 or USB) can be integrated. The control software is a web application that enables real-time signal collection and stabilization. Consequently, both kinetic and titration data are obtained and saved as files. As a proof of concept, the standardization of hydroxide and thiosulfate solutions was performed with precision better than 2%.
[1] Oliveira et al.Quim.Nova, 33(3):721-724.

Agradecimentos/Acknowledgments

The authors thank the UFV/CISAB-ZM Research Agreement for the financial support of this research

Avaliação da composição química elementar de cumaru (Dipteryx odorata (Aubl.) Willd.))

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Palavras Chave:*elementos essenciais, elementos tóxicos, controle de qualidade,cumaru, elementos essenciais, elementos tóxicos, controle de qualidade*

Highlights

Cumaru is rich in coumarin and increasingly consumed, but data on essential and toxic elements are limited. So, it was determined As, Cd, Ca, K, Mg, Cu, Fe, Zn, Se, P, Pb, and S by ICP OES.

Resumo/Abstract

Cumaru (*Dipteryx odorata*(Aubl.) Willd.) apresenta uma grande importância ecológica e comercial, sendo utilizado como principal fonte de renda no norte do Brasil. Pertencente à família Fabaceae, esta espécie destaca-se tanto pelo valor econômico da madeira quanto pelas propriedades aromáticas e bioativas de suas sementes, tradicionalmente utilizadas na perfumaria, farmacologia e culinária. O cumaru é reconhecido principalmente pela presença de cumarina, um heterocíclico orgânico de intensa fragrância e diversas propriedades farmacológicas, como atividade anticoagulante, antioxidante, anti-inflamatória, antibiótica e antimicrobiano. Diante das propriedades terapêuticas do cumaru, o crescimento do seu consumo torna-se necessário um maior controle de qualidade, principalmente de sua composição química elementar, uma vez que há uma escassez de informações a respeito da concentração de elementos essenciais e tóxicos. Diante disso, este trabalho está avaliando a composição química elementar de sementes de cumaru, determinando concentração de elementos essenciais (Ca, K, Mg, Cu, Fe, Zn, Se, P e S) e tóxicos (As, Cd e Pb) por ICP OES. As amostras estão sendo submetidas à digestão ácida com mistura oxidante diluída e aquecimento por micro-ondas. Teste de adição e recuperação será aplicado para avaliação de interferência químicas na determinação elementar por ICP OES. Pretende-se desenvolver procedimentos que auxiliem a análise química de alimentos importantes nacional e internacionalmente. Além de fornecer informações nutricionais e tóxicas de uma semente pouco estudada, mas com grande interesse terapêutico pela população que a consome.

Agradecimentos/Acknowledgments

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Avaliação de Resíduos da produção de chá na extração em fase sólida de Cádmio em corpos hídricos

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Palavras Chave:*Cádmio,Extração em fase sólida,Adsorvente Sustentável,Química Verde*

Highlights

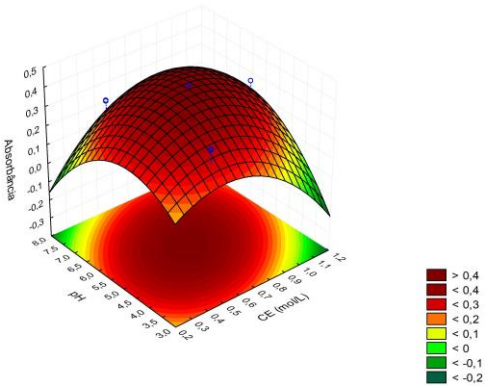
Tea residues remove Cd^{2+} from water efficiently. The method allows sensitive analysis in aquatic media, uniting waste recovery with green and sustainable chemistry.

Resumo/Abstract

A contaminação de corpos hídricos por metais potencialmente tóxicos representa um grave risco ambiental e á saúde humana, devido á sua persistência e capacidade de bioacumulação. Dentre esses metais, o Cádmio destaca-se por sua elevada toxicidade mesmo em baixas concentrações. Neste trabalho, avaliou-se o uso de resíduos da produção de chá como material adsorvente (Tads) na extração em fase sólida de Cd^{2+}, visando o desenvolvimento de uma alternativa sustentável, de baixo custo e alinhada aos princípios da Quimica Verde. O material adsorvente foi preparado a partir de resíduo de chá seco e pulverizado, acondicionado em mini coluna acoplada a um sistema de analise por injeção em fluxo(FIA) como detecção por espectometria de absorção atômica em chama(FAAS). A caracterização morfologica por microscopia eletrônica de varredura(MEV) evidenciou superfície rugosa e estrutura fibrosa típica de materiais lignocelulósicos, enquanto a análise por espectroscopia de energia dispersiva de raios X(EDS) confirmou a predominância de C e O, além da presença de grupos funcionais favoráveis á adsorção de íons metálicos. As variáveis químicas e de fluxo foram otimizadas por planejamento fatorial 2^3 e Matriz de Doehlert, sendo definidas como condições ótimas pH 5,5, e concentração do eluente (HNO_3) de 0,7 mol L^{-1} e vazão de pré-concentração de 7,5 mL min^{-1}. O sistema apresentou fator de enriquecimento de 16,6, com redução significativa dos limites de detecção e quantificação para Cd^{2+}. Os resultados obtidos até o momento apontam que o TAds, obtido de resíduo vegetal, demonstrou alta eficiência na retenção de cádmio, atribuída aos seus grupos funcionais ativos. Trata-se de um material verde, de baixo custo e sustentável, alinhado à Química Verde e à Economia Circular, com grande potencial para aplicações ambientais.

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Superfície de resposta e vista via curva de nível obtidas pela Matriz de Doehlert relacionando pHxCE

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Best Practices in Untargeted LC-MS Metabolomics for Robust and Reproducible Biomedical Research

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Palavras Chave:*LC-MS,Method Optimization,Sample Preparation,Quality Control,Animal Models*

Highlights

We address critical analytical gaps in untargeted metabolomics by systematically evaluating key parameters and defining best practices to reduce technical noise and reveal true biological variation.

Resumo/Abstract

Robust biomedical research, fundamental to national health sovereignty, requires analytical tools that deliver reliable biological insights. Untargeted metabolomics is a powerful approach for investigating disease models and therapeutic responses; yet its reliability depends on a meticulously optimized workflow, from sample preparation to data acquisition. Inconsistent methods can obscure real biological variation by technical noise. This work presents a systematic study to establish best practices for untargeted LC-MS metabolomics. Using mouse liver as a model, we evaluated four extraction protocols (varying solvent systems and tissue disruption methods) and analyzed each under four complementary LC-MS conditions: reversed-phase and hydrophilic interaction liquid chromatography, each employing positive and negative electrospray ionization modes. Pooled quality control (QC) samples were used to monitor analytical stability. Our data reveal critical trade-offs: biphasic extraction increased signal intensity but also introduced greater inter-sample variability, illustrating a precision-for-sensitivity balance. Tissue maceration had a less pronounced effect on feature counts. The orthogonal LC-MS conditions were essential for comprehensive metabolome coverage, enabling the detection of distinct compound classes. QC samples proved vital for assessing reproducibility and enabling robust normalization to correct for instrumental drift. Furthermore, we implemented an intelligent data-dependent acquisition strategy using dynamic exclusion lists, significantly increasing the number of high-quality MS/MS spectra for confident metabolite annotation. This study provides an evidence-based framework for designing untargeted metabolomics experiments. By understanding the impact of each analytical step, researchers can make informed choices to enhance data quality. We advocate these optimized practices as a fundamental standard to advance reliable translational biomedical research.

Agradecimentos/Acknowledgments

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Beyond Prediction: Interpretable Machine Learning as a New Paradigm in Chemometrics

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Palavras Chave:*Interpretable Machine Learning; Chemometrics; Explainable Artificial Intelligence (XAI); Benchmark Datasets; Predictive Modeling*

Highlights

Interpretable ML models improve the transparency of chemometrics predictions. SHAP-based analysis reveals the key variables that drive chemical classification and regression models.

Resumo/Abstract

Machine learning is rapidly transforming chemometrics by enabling predictive modeling of complex multivariate systems. However, the increasing use of highly accurate yet opaque algorithms challenges one of the central goals of chemometrics: extracting scientific knowledge from data. Interpretable Machine Learning (IML) offers a principled approach that combines predictive performance with quantitative model transparency.
In this work, interpretable machine learning is introduced as a core component of the chemometric workflow rather than as a post hoc diagnostic tool. Using the publicly available Boston Housing dataset as a benchmark for multivariate regression, we demonstrate how explainability methods can reveal the internal structure of predictive models and quantify variable influence in a rigorous, reproducible manner. The dataset provides a controlled environment for evaluating interpretability strategies applicable to chemical and analytical datasets.
Supervised learning models were developed and interpreted using feature-importance analysis and SHAP (Shapley Additive Explanations) values, enabling both global and local interpretation of predictions. The results show that interpretable models can simultaneously achieve high predictive performance and provide meaningful insight into variable contributions, model sensitivity, and prediction logic.
The proposed framework advances chemometrics by repositioning interpretability as a fundamental objective of modeling. By integrating explainable AI into predictive workflows, this study establishes a reproducible paradigm for transparent machine learning in chemical data analysis. This contribution supports the transition from black-box prediction to knowledge-driven chemometric modeling.

Agradecimentos/Acknowledgments

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Biomonitoring of trace elements in humans: possible biomarkers in chronic non-communicable diseases.

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Palavras Chave:*Biomonitoring,Biomarkers,Chemical Speciation,Analytical Chemistry*

Highlights

Biomonitoring studies can provide essential information for understanding the mechanisms of diseases and their relationship with trace elements.

Resumo/Abstract

The biomonitoring of inorganic elements represents an essential frontier in analytical chemistry, serving as a high-precision tool for identifying biomarkers for non-communicable chronic diseases (NCDs). By utilizing advanced spectrometric techniques and chemical speciation, it is possible to assess more than the determination of total concentrations and achieve an understanding of the biologically active and potentially toxic fractions present in complex matrices. Large-scale biomonitoring studies in Latin America are still few. In Fortaleza, Ceará, some studies are being developed with school populations in the search for inorganic biomarkers for chronic diseases such as obesity, malnutrition, and hidden hunger. Furthermore, it is possible to obtain inorganic markers for problems such as high blood pressure, cancer, and other metabolic disorders. These studies can also be aligned with specific questionnaires to help us to understand the role of external factors such as diet, occupation, and other factors in exposure to toxic and/or essential elements. Biomonitoring is essential to evaluate oxidative stress markers that are mainly related to elements such as Cu, Fe, Se, and Zn, which are cofactors of antioxidant enzymes. Their imbalance has been found in some populations studied by the group, with special attention to pregnant women with pre-eclampsia, in the differentiation of thyroid nodules, and in childhood obesity. In these types of studies, analytical chemistry plays an essential role in solving analytical problems to obtain more precise information, such as the analysis of halogens in biological tissue, the analysis of toxic elements, and chemical speciation, which can provide essential information to unravel the function of these elements in human metabolism. In this regard, important results from biomonitoring programs will be presented, focusing on the search for inorganic biomarkers for NCDs and the role of analytical chemistry in this process.

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CHARACTERIZATION OF DIAMONDOIDS IN CRUDE OIL BY LPGC-MS/MS

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Palavras Chave:*Low-pressure Gas Chromatography, Mass Spectrometry, Diamondoids, Crude Oil, Fast Analysis*

Highlights

Diamondoids are highly stable biomarkers crucial in petroleum studies, resistant to thermal and microbial alteration.
This study proposes a high-throughput method preserving chromatographic resolution.

Resumo/Abstract

Diamondoids are alkanes with a diamond-like structure and have been detected in crude oil. Adamantane and diamantane are key compounds representative of two homologous series within this group. Due to their high thermal stability and resistance to microbial attack, diamondoids are potential biomarkers for diagnosing petroleum origin and geologic history. Biomarker profiling is typically performed using gas chromatography coupled to tandem mass spectrometry (GC-MS/MS), but conventional methods require high peak capacity and long run times. This study aims to improve the characterization of diamondoids in crude oil by developing a faster method that maintains chromatographic resolution. To achieve this, vacuum outlet conditions were coupled with a short, wide-bore column (also known as low-pressure gas chromatography, or LPGC) to increase analysis speed. In essence, the viscosity of the carrier gas is lower at lower pressures than at higher pressures, which shifts the optimum linear flow velocity in the Golay equation to a higher flow rate, reducing analysis time and maintaining an acceptable degree of separation. The compounds of interest are located within the saturated fraction. An important preparative step involved separating the sample into saturated, aromatic, resinous, and asphaltenic fractions (SARA) using open-column liquid chromatography.
The target fraction was subsequently analyzed by LPGC–MS/MS in Selected Ion Monitoring (SIM) and Selected Reaction Monitoring (SRM) modes, monitoring molecular-to-product ion transitions (e.g., $M^{\bullet+} \rightarrow 135$ for methyl-adamantanes and $M^{\bullet+} \rightarrow 187$ for methyl-diamantanes). Comparisons with GC were conducted, and experimental parameters, such as carrier gas flow and temperature programming, were optimized to ensure maximum chromatographic resolution and identification of the main diamondoids. As a result, analysis time was reduced by approximately 5x.

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CAPES, CNPq, FAPESP, Petrobras

Characterization of Ricin-Galactose Interaction through NMR Spectroscopy

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Palavras Chave:*Ricin,NMR,Galactose,Protein-Ligand Interaction*

Highlights

Investigation of Ricin B-chain lectin activity by NMR.
NMR mapping of galactose binding epitopes.
Structural insights into toxin-carbohydrate recognition.

Resumo/Abstract

Ricin is a potent toxin from*Ricinus communis*and a significant concern in toxicology and biodefense. Its extreme toxicity is exacerbated by the lack of approved therapeutic antidotes. As a Type II ribosome-inactivating protein (RIP), Ricin relies on a heterodimeric structure for its mechanism of action. The A-chain provides enzymatic activity, while the B-chain (RTB) acts as a lectin to mediate cell entry. Specifically, the RTB binds to terminal galactose and N-acetylgalactosamine residues of glycoproteins and glycolipids displayed on the cell surface.
In this study, NMR spectroscopy is used to map the binding epitopes of galactose interacting with RTB in aqueous solution. Saturation Transfer Difference (STD) NMR is a robust, ligand-observed technique. It identifies the binding epitope by measuring saturation transfer from the protein receptor to ligand protons in the bound state. This methodology provides a detailed map of ligand segments in direct contact with the binding pocket. Such insights clarify the biophysical parameters governing Ricin's initial docking stages. Furthermore, these data support the design of specific carbohydrate-based inhibitors, fostering technological autonomy and national sovereignty.

Agradecimentos/Acknowledgments

To the Military Institute of Engineering and the Institute of Chemical, Biological, Radiological and Nuclear Defense for providing the infrastructure necessary for the development of this work.

Comparative Determination of Iron in Pereskia Species using ICP-OES: A Study on Nutritional Potential

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Palavras Chave:*Pereskia,Ferro,ICP-OES,Liofilização,PANCs*

Highlights

ICP-OES with In internal standard identifies P. bleo as a rich Fe source (165 mg kg⁻¹). Lyophilization maximizes recovery, proving pre-treatment is essential for accurate mineral analysis.

Resumo/Abstract

The genus Pereskia (Cactaceae), popularly known as "ora-pro-nobis," is a Non-Conventional Food Plant (PANC) recognized for its high nutritional value, particularly as a source of iron (Fe) to combat mineral deficiencies. This study evaluated the Fe content in three species—Pereskia aculeata mill (PAM), Pereskia grandifolia (PG), and Pereskia bleo (PB)—comparing the effects of oven drying (45 °C) and freeze-drying (lyophilization) on the final quantification.

Approximately 0.2000 g of sample underwent microwave-assisted acid decomposition using a mixture of 3.00 mL HNO_3, 3.00 mL H_2O, and 2.00 mL H_2O_2 (30% m m^{-1}). Following a 30 min pre-decomposition period, the heating program consisted of 10 min to 100 °C (10 min hold) and 10 min to 180 °C (10 min hold), with final solutions diluted to 15 mL. Fe was determined using ICP-OES under 1300 W radiofrequency power, with gas flows of 15 L min^{-1} (plasma), 0.2 L min^{-1} (auxiliary), and 0.80 L min^{-1} (nebulization) at a sample flow of 1.50 mL min^{-1}. Measurements utilized axial view at 259.939 nm. To ensure analytical accuracy and correct instrumental fluctuations, Indium (In) at 371.029 nm was employed as an internal standard with a dilution factor of 10. The method demonstrated high reliability, with a linearity (R^2) of 0.99990 and a limit of quantification for Fe of 11 mg kg^{-1}. The results revealed that Pereskia bleo (PB) has the highest Fe concentration, reaching 165 ± 5 mg kg^{-1} when freeze-dried, significantly higher than PG (79 ± 9 mg kg^{-1}) and PAM (106 ± 26 mg kg^{-1}). Student's t-test ($p < 0.05$) showed that PB was the only species where the drying procedure significantly influenced Fe determination, with lyophilization yielding higher recovered concentrations compared to oven drying (128 ± 7 mg kg^{-1}). These findings highlight the importance of species selection and pre-treatment optimization for accurate nutritional characterization.

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Agradecimentos/Acknowledgments

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Comparison of parametric and permutation t-spectral representations for metabolite discrimination in factorial NMR designs

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Palavras Chave:*Metabolomics,NMR spectroscopy,Factorial design,Permutation tests,Statistical validation*

Highlights

Parametric and permutation t-spectral representations were compared. Permutation tests validated all significant parametric peaks. No additional metabolites were revealed by permutation analysis.

Resumo/Abstract

Two-level factorial design spectra can be transformed into t-spectral representations to investigate individual metabolite abundance changes associated with environmental effects. These representations are obtained by calculating statistically paired t-values for each spectral variable, allowing direct interpretation of metabolic variations across experimental factors. However, parametric t-tests rely on assumptions of normality and variance homogeneity, which may not always be satisfied in high-dimensional spectroscopic data. In this study, parametric and permutation-based t-spectral representations were compared using ^{1}H NMR spectra from ethanol, dichloromethane, and ethanol–dichloromethane (1:1) extracts of*Ilex paraguariensis*leaves. The data were obtained from a balanced 2^2 factorial design evaluating sexual dimorphism and light incidence effects, comprising 13,501 spectral variables. Permutation calculations with up to 100,000 iterations were applied to estimate statistical significance without relying on parametric assumptions. All metabolite peaks identified as statistically significant by parametric t-calculations were confirmed by permutation analysis, and no additional significant peaks were detected. Root mean square errors between parametric and permutation t-values were low, demonstrating strong agreement between methods. Deviations were observed only for highly significant peaks, reflecting the intrinsic sensitivity of t-values at extreme significance levels. Permutation testing proved particularly useful for spectral regions exhibiting variance heterogeneity according to Bartlett's test. These results demonstrate that permutation-based t-spectral representations provide robust validation of parametric findings and are recommended for reliable interpretation of metabolomic data obtained from balanced factorial designs.

Agradecimentos/Acknowledgments

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Comparison of SPE and SLE for the Characterization of Bio-oil Aqueous Phases from Sugarcane Bagasse and Textile Sludge via GC×GC-TOFMS

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Palavras Chave:*Bio-oil, GC×GC-TOFMS, Aqueous phase, Extraction methods, Textile sludge*

Highlights

SLE effectively extracts low-polarity species;

SPE favors high-polarity compounds like levoglucosan;

Textile sludge acts as a deoxygenating catalyst in sugarcane bio-oil blends.

Resumo/Abstract

The global energy transition highlights the importance of lignocellulosic biomass, particularly sugarcane bagasse (SCB), for bio-oil production via pyrolysis. However, the aqueous phase of bio-oil comprises up to 70% of the liquid product of pyrolysis and exhibits high acidity and water content, necessitating detailed characterization for valorization. This study aims to characterize the chemical profile of SCB bio-oil aqueous phases using comprehensive two-dimensional gas chromatography (GC×GC-TOFMS). Extraction techniques, such as solid-phase extraction (SPE) and supported liquid extraction (SLE), were evaluated for the efficient extraction of organic compounds from aqueous matrices, and the catalytic effect of adding 50% waste textile sludge (WTS) to sugarcane bagasse (SCB) was examined. Results showed that the SLE protocol was superior for extracting low-polarity compounds such as acids, alcohols, furans, and indenes. SPE was more efficient in extracting high-polarity species, notably hexoses, such as levoglucosan. Tile-based chemometric analysis was applied to identify discriminant compounds. The Fisher ratio was used to select relevant tile regions, revealing acetic acid as a descriptor of SLE samples and 3-hydroxypropyl-oxirane as characteristic of SPE samples. Regarding the catalytic effect, the addition of 50% WTS significantly reduced the concentration of oxygenated compounds in the aqueous phase. Although WTS introduced nitrogen and sulfur species from its matrix, the SLE-SCB+WTS 50% samples exhibited the highest potential for energy applications due to the reduction in oxygenate levels. Also, the SPE-SCB route proved ideal for recovering of platform molecules like phenolics. The combination of extraction methods and GC×GC-TOFMS provided a deep understanding of the bio-oil aqueous phase, supporting circular-economy models by valorizing agricultural and industrial residues into valuable chemical resources.

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COMPUTATIONAL APPROACH TO NPS IDENTIFICATION: INTEGRATION OF THEORETICAL IR SPECTROSCOPY AND ARTIFICIAL INTELLIGENCE

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Palavras Chave:*Benzodiazepines,Opioids,infrared spectroscopy,Machine learning,Infrared spectroscopy*

Highlights

Machine learning was applied to verify classification
Unsupervised techniques successfully grouped classes
Shallow-ANN failed and Deep-ANN converged the correct prediction

Resumo/Abstract

Identifying New Psychoactive Substances (NPS) is challenging due to their structural diversity, rapid market emergence, and limited spectral references. These issues hinder analytical workflows, especially for benzodiazepine- and opioid-type NPS. Computational methods like spectroscopy and machine learning can predict spectral behavior and classify new substances even before reference standards exist. This study used unsupervised and supervised machine learning to characterize novel benzodiazepines and opioids. IR spectra were simulated via Density Functional Theory (DFT) in ORCA. Unsupervised analysis—Hierarchical Cluster Analysis (HCA) and Principal Component Analysis (PCA)—investigated natural groupings among molecules. Supervised models, including shallow and deep Neural Networks (NNs), predicted classes from IR-spectrum features in RStudio. They were validated by comparing theoretical spectra with experimental IR data from SWGDRUG. PCA and HCA effectively clustered benzodiazepines and opioids based on spectra, showing strong grouping. Shallow NNs had limited discrimination, despite tuning, producing 'flattened' outputs near 0 or 1 that missed subtle spectral differences. A deep neural network with three hidden layers (10–50–10 neurons), trained for 50 epochs at a 0.01 learning rate using sigmoid activation, improved classification. Applying a threshold separated classes clearly. The neural network achieved about 80% accuracy for benzodiazepines and 90% for opioids when matching theoretical to experimental spectra. This work highlights the value of combining machine learning with theoretical spectroscopy for NPS identification. Unsupervised methods reliably cluster, while deep neural networks are key for accurate classification and validation against experimental data. Future studies will extend this framework to more NPS classes and complex multi-class scenarios.

Agradecimentos/Acknowledgments

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Cultivo de cebolinha (Allium schoenoprasum L.) contaminado com cádmio: efeito na distribuição de elementos essenciais

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Palavras Chave:*cádmio, cebolinha, hidroponia, elementos essenciais*

Highlights

The elemental enrichment strategy should be seen as an alternative to reduce environmental contamination. For this, the study evaluated the cadmium effect on the distribution of essential elements.

Resumo/Abstract

A cebolinha (*Allium fistulosum*L.) é uma hortaliça de fácil cultivo, inclusive o hidropônico, e bastante benéfica quando visa-se alcançar uma dieta saudável, pois fornece diversas vitaminas, fibras e elementos essenciais (K, Mg, Ca e P). A hidroponia permite o enriquecimento elementar de cebolinha, mas deve ser vista além da necessidade de suprir deficiências nutricionais, uma vez que é possível também ser aplicada na resolução de problemas ambientais. Utilizar procedimentos de enriquecimento para fins de diminuição de toxicidade por elementos tóxicos em alimentos requer estudos de interações entre os diferentes elementos durante a absorção e translocação. Desta forma, fica evidente que para o sucesso de procedimentos de enriquecimento, visando melhoramento nutricional ou minimização/eliminação de problemas de toxicidade por metais pesados, estudos de competição entre elementos são de suma importância. Logo, este trabalho avaliou o efeito da contaminação de cádmio durante o cultivo hidropônico de cebolinha na distribuição de elementos essenciais (Ca, Cu, Fe, P, S, Se e Zn) por ICP OES. As condições de cultivo foram estudadas e soluções de 1, 10 e 100 μg L^{-1} Cd(II) foram aplicadas para induzir contaminação. Após 14 dias de cultivo, as folhas foram cortadas, secas e moídas. Para a análise por ICP OES, as amostras serão submetidas a digestão com mistura oxidante diluída e aquecimento em forno de micro-ondas. Teste de adição e recuperação será feito para verificar a existência de interferências químicas. Comparações com o grupo controle (não enriquecido) serão feitas para verificar o efeito da contaminação na distribuição dos elementos essenciais.

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Desenvolvimento de Protótipo usando Lã de PET como adsorvente na remoção de microplásticos em corpos hídricos: estudos iniciais para Tecnologia Social

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Palavras Chave:*Microplásticos; Lã de PET; Adsorvente; corpos hídricos; Tecnologia Social.*

Highlights

"A prototype using recycled PET wool adsorbs up to 90% of microplastics in water samples, offering a low-cost solution with potential as a social technology."

Resumo/Abstract

Os microplásticos (MP) representam um dos principais desafios ambientais da atualidade devido à sua persistência e aos impactos ecológicos e à saúde humana[1]. São definidos como fragmentos plásticos menores que 5 mm[2]. O poli(tereftalato de etileno) (PET) apresenta leveza, resistência química e estabilidade física, propriedades que favorecem sua aplicação na remoção de MP da água, alinhando-se aos princípios da economia circular e da mitigação sustentável de poluentes[3]. Os microplásticos foram adquiridos de uma empresa de reciclagem e separados por peneiramento (malhas Tyler de 75, 106 e 212 µm). A lã de PET, utilizada como isolante acústico, foi empacotada em colunas de adsorção de 5 e 100 mL. As suspensões de MP foram percoladas pelas colunas, coletando-se alíquotas antes e após o processo para análise qualitativa por estereomicroscopia e quantitativa por rastreamento de nanopartículas (NTA, sistema ZetaView). Para maior uniformidade experimental, foram utilizadas partículas <106 µm, devido à sua relevância ambiental e maior potencial de interação com compartimentos biológicos. A caracterização por Microscopia Eletrônica de Varredura (MEV) revelou partículas com morfologia irregular, superfícies rugosas e elevada resistência, características que aumentam a área de contato e favorecem a adesão às fibras de PET. A natureza hidrofóbica dos MP pode intensificar interações físicas e químicas com os grupos éster do PET, contribuindo para maior retenção. As análises de MEV da lã de PET evidenciaram fibras finas e entrelaçadas, com boa permeabilidade, favorecendo mecanismos de retenção por peneiramento, enredamento e interações hidrofóbicas. Ensaios qualitativos foram realizados com soluções contendo 10 e 25 mg/50 mL de MP (<106 µm), percoladas em coluna de 100 mL a 13,5 mL min^{-1}. Observou-se redução significativa da concentração de partículas após a passagem pela coluna. A análise por NTA indicou eficiência de retenção aproximada de 90%, com redução da concentração de 1,2 × 10^8 para 1,2 × 10^7 partículas mL^{-1} após o tratamento, confirmando quantitativamente o desempenho adsortivo. Os resultados demonstram o potencial da lã de PET reciclada como alternativa sustentável, de baixo custo e amplamente disponível para mitigação da poluição por microplásticos em ambientes aquáticos.

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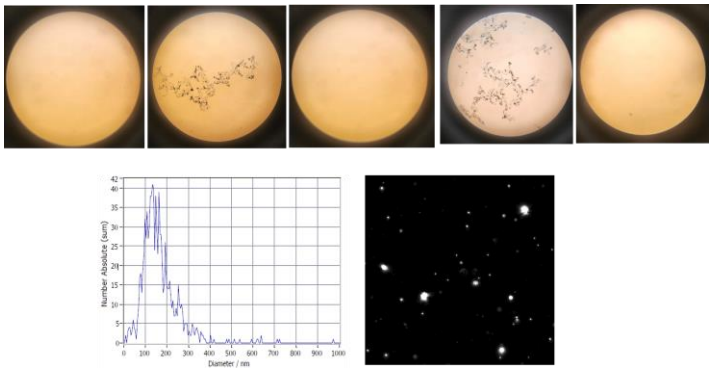


Figura: Esteriomicroscopia das soluções de MP antes e após passar pela coluna de 100 ml de lã de PET

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DESENVOLVIMENTO DE UM TITULADOR AUTOMÁTICO EM FLUXO CONTÍNUO PARA TITULAÇÃO POTENCIOMÉTRICA

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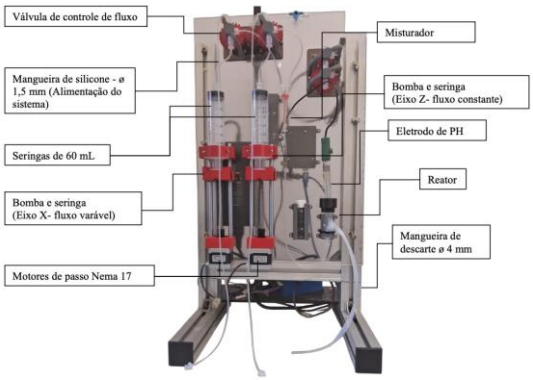
Palavras Chave:*Titulação Potenciométrica,Análise por injeção em fluxo,arduino,Interpolação helicoidal,Automação*

Highlights

Continuous-flow potentiometric titrator using low-cost syringe pumps and valves and open-source electronics. pH vs. time with a sigmoidal fit validated the HCl/NaOH titration with a 2.7% error.

Resumo/Abstract

Este trabalho descreve o desenvolvimento de um titulador automático operando em fluxo contínuo, baseado na técnica de análise por injeção em fluxo (FIA, do inglês *Flow Injection Analysis*), para a realização de titulações potenciométricas de forma automatizada. O dispositivo emprega duas bombas de seringa e duas válvulas de três vias, acionadas por motores de passo e controladas por um microcontrolador Arduino Mega executando firmware Marlin. As válvulas de três vias foram construídas com engrenagens de dentes helicoidais duplos, impressas em impressora 3D, para coordenar o direcionamento do fluxo dos reagentes. O controle de fluxo utilizou interpolação helicoidal via firmware Marlin, de modo a decompor a velocidade tangencial do sistema em componentes vetoriais. Essa estratégia permite que uma seringa opere com vazão constante enquanto a outra gera um gradiente de concentração variável. O monitoramento do pH foi realizado com um sensor de pH modelo 4502C acoplado a um Arduino Uno, e a aquisição de dados foi gerenciada por um software desenvolvido em Python. O tempo total de titulação foi de 523,60 s, sendo o método baseado na medição de pH em função do tempo. Para mitigar ruídos instrumentais e identificar o instante do ponto de equivalência, os dados brutos foram submetidos a um ajuste sigmoidal. Os tempos de ponto de equivalência, em triplicata, foram 285,37; 284,17; e 293,94 s. A validação do sistema foi realizada pela titulação de uma solução padronizada de HCl (0,0498 mol L^{-1}) com NaOH (0,0503 mol L^{-1}). Os resultados indicaram concentração média experimental de 0,0485 ± 0,0007 mol L^{-1} (95% de confiança), desvio padrão de 0,0003 mol L^{-1} e erro relativo de 2,7%. O sistema desenvolvido possibilitou a execução automatizada do processo de titulação nas condições experimentais estabelecidas.



Vista geral do dispositivo de titulação automática em fluxo contínuo.

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Desenvolvimento e Validação de Método Analítico para Compostos Furânicos: Síntese e Otimização do Ácido Levulínico a partir de amido

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Palavras Chave:*Biorrenováveis Biomassa,Química verde; Planejamento fatorial e Sustentabilidade.,Biorrenováveis ; Biomassa,Química verd Planejamento fatorial e Sustentabilidade.,Biorrenováveis*

Highlights

Conversão de amido em ácido levulínico via LiBr MSH como rota sustentável de valorização da biomassa. Desenvolvimento e validação de método GC-MS para compostos furânicos conforme RDC nº 166/17.

Resumo/Abstract

A busca por alternativas sustentáveis tem impulsionado o desenvolvimento de processos químicos a partir de biomassa, um recurso renovável rico em carbono. A conversão de biomassa em compostos de alto valor agregado, como o ácido levulínico (AL) é promissora devido a diversas aplicações nas indústrias farmacêutica, cosmética, alimentícia e de biocombustíveis. Embora diferentes tipos de biomassa, como celulose e lignocelulose, tenham sido amplamente estudados, a conversão do amido utilizando LiBr MSH (do inglês Lithium Bromide Molten Salt Hydrates) trata-se de uma abordagem promissora pouco explorada, especialmente quanto à otimização das condições reacionais e compreensão dos mecanismos envolvidos. Sendo assim, este projeto tem como objetivo desenvolver e validar um método analítico por GC-MS (do inglês Gas Chromatography–Mass Spectrometry) para a quantificação de compostos furânicos, conforme a RDC no 166/17. Além disso, visa realizar a síntese de ácido levulínico a partir do amido em hidratos de sais fundidos de brometo de lítio, com otimização por meio de DoE (do inglês Design of Experiments). A proposta representa um avanço na área de biorrefinaria ao consolidar estratégias inovadoras para a valorização sustentável da biomassa, viabilizando alternativas para a redução da dependência de recursos fósseis e mitigando impactos ambientais.

Agradecimentos/Acknowledgments

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Determination of chemical attribution signatures of nerve agent precursors by GC–MS and GC coupled to element-selective detectors

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Palavras Chave:*Chemical attribution signares,Chemical warfare agents,Chemical forensics,Impurity profiling*

Highlights

GC techniques enable impurity profiling of nerve agent precursors for forensic attribution under the Chemical Weapons Convention.
Multivariate statistical analysis differentiates sample origins.

Resumo/Abstract

The use of toxic chemicals as warfare agents led to the establishment of the Chemical Weapons Convention (CWC) and the Organization for the Prohibition of Chemical Weapons (OPCW), which coordinates an international network of designated laboratories responsible for chemical identification and verification. Within this framework, chemical forensics plays a central role in investigations related to the origin, production, and potential misuse of such prohibited substances. Among those compounds, organophosphorus nerve agents and their precursors are of particular relevance, as their synthesis, storage, and degradation generate characteristic impurity patterns that can be exploited as chemical attribution signatures of forensic interest.
In this study, analytical methodologies based on gas chromatography coupled to mass spectrometry (GC–MS) and element-selective detectors (GC-NPD/FPD) were applied to the characterization of impurity profiles of O,O-diethyl methylphosphonate (DEMP), a nerve agent precursor with both industrial relevance and regulatory importance under the CWC. Commercial and in-house synthesized samples were analyzed under identical analytical conditions to construct representative impurity profiles.
Data obtained by GC–MS and GC-NPD/FPD were processed and combined using data fusion strategies to enhance pattern recognition and sample discrimination. Similarity and selectivity metrics were calculated, followed by multivariate statistical analysis using principal component analysis (PCA) and partial least squares analysis (PLS). The results indicate that this approach enables the differentiation of samples according to their synthetic origin, supporting forensic attribution and strengthening verification activities under the CWC, while contributing to Brazil's national sovereignty by enabling responsibility attribution in cases of potential unauthorized use of such chemicals.

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Determination of enzymatic activity using smartphone-based digital video

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Palavras Chave:*Smartphone,Enzyme activity,Green Analytical Chemistry,Digital-image photometry*

Highlights

Novel approach for determination of enzymatic activity; Results in agreement with UV-Vis spectrophotometric method (Er = -2%); Simple, low-cost, and green alternative (waste volume < 2 mL).

Resumo/Abstract

Enzyme activity is usually determined by monitoring either substract or reaction product over a fixed time, but the approach is limited by the need for reaction-time control. Urease catalyses the hydrolysis of urea into ammonia and carbon dioxide, playing a key role in the nitrogen cycle, and being relevant in environmental and clinical applications. Its activity is typically measured by ammonium determination using colorimetric methods or steam distillation, but these approaches show low greenness (AGREE 0.40 and 0.27) due to toxic reagents, high waste generation, and low sample throughput. Here, we developed a practical approach for enzymatic activity determination exploring digital videos, taken urease as a model. The method indirectly monitors urea hydrolysis through the phenol red color changes caused by ammonia formation. Analytical-grade reagents were used, including jack bean (Canavalia ensiformis) urease. Digital videos were recorded for 10 min under controlled lighting, and analytical information corresponding to the alkaline form of phenol red (maximum absorption at 550 nm) was obtained from channel G of the RGB color system. Frames were extracted every 10 s and processed in ImageJ using in-house Python software. A calibration curve was constructed by varying the phenol red concentration within a range that did not affect the solution pH. Urease activity was calculated from the reaction rate ($\Delta G/t$), where $\Delta G = G - G_0$ and t is the time required to reach the reaction plateau (5 min). The urease activity determined by the smartphone-based method using 60 mg L-1 urea was 0.138 ± 0.001 U mL-1, compared with 0.141 ± 0.001 U mL^{-1} obtained by UV-Vis spectrophotometry, resulting in a relative error of -2%. This agreement demonstrates the suitability of digital video photometry for urease activity determination and supports its application as a simple, cost-effective alternative that reduces waste volume to 2 mL, contributing to an AGREE score of 0.77.

Agradecimentos/Acknowledgments

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Determination of Iodine in Thyroid Nodules by ICP-MS: A possible biomarker for nodule malignancy

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Palavras Chave:*Halogen,Thyroid Cancer,ICP-MS*

Highlights

For the first time, iodine levels were quantified in human thyroid tissue using ICP-MS. Iodine levels were higher in atypical nodules than in benign and high-probability malignant categories.

Resumo/Abstract

The determination of iodine is fundamental for understanding thyroid pathophysiology. However, its quantification in biological tissues is analytically challenging due to halogen volatility and matrix effects. This study aimed to compare iodine concentrations in thyroid tissue with nodules according to cytological classification and to evaluate its potential as a complementary biomarker. This cross-sectional study included 26 individuals. Blood samples were collected for thyroid hormones (T3, T4, and TSH) and antioxidant enzymes quantification. For iodine determination, thyroid tissue samples were decomposed by microwave-induced combustion (MIC). Freeze-dried samples were wrapped in filter paper moistened with 50 µL of 6.0 mol L^{-1} NH_3NO_3 and combusted in quartz vessels containing 6.0 mL of 150 mmol L^{-1} NH_4OH as the absorbing solution, under 20 bar of O_2. Iodine was determined by ICP-MS. The trueness of the method was evaluated using NIST 1566b (Oyster Tissue) with 94.5% of recovery. All results are expressed in dry mass.

Higher iodine concentrations were observed in tissue adjacent to nodules classified as Bethesda III (8071 µg g^{-1}), possibly reflecting adaptive responses to oxidative stress due to the antioxidant role of iodine, compared with Bethesda II (3405 µg g^{-1}), where preserved iodine uptake suggests maintained thyroid functionality, and Bethesda IV/V (2512 µg g^{-1}), in which reduced iodine levels may indicate impaired iodide transport associated with cellular differentiation. No statistically significant differences were observed in serum thyroid hormone levels, showing the importance of iodine quantification as a biomarker of malignancy. Nevertheless, the levels of oxidative stress related to the activity of SOD (2817.9 U gHb^{-1}) and GPx (281.9 U gHb^{-1}) are higher than the clinical normal levels (1102–1601 U gHb^{-1} for SOD and 27.5–73.6 U gHb^{-1} for GPx), suggesting a persistent pro-oxidative environment due to the relation of iodine in this mechanism.

Agradecimentos/Acknowledgments

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Determination of Mercury and Health Risk Assessment in Fish Consumed by the Cajueiro Community on Mosqueiro Island (PA)

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Palavras Chave:*Metal toxic,Mercury,Bioaccumulation,Amazon,Exposure risk assessment.*

Highlights

Determination of total mercury in three fish species; human health risk indices are evaluated and discussed; analysis of mercury concentrations using the DMA-80 analyzer.

Resumo/Abstract

Riverside communities in the Amazon region rely heavily on artisanal fishing as a primary source of protein and income, making the monitoring of environmental contaminants such as mercury essential for food safety [3]. This study aimed to determine total mercury (THg) concentrations in fish consumed and commercialized in the Cajueiro community, located on Mosqueiro Island (Belém City, Pará State, Brazil), and to assess the potential human health risks associated with fish consumption. A total of 12 samples from three fish species were analyzed: piramutaba (*Brachyplatystoma vaillantii*), sarda (*Sarda sarda*), and white croaker (*Plagioscion squamosissimus*). Total mercury concentrations were determined using atomic absorption spectrometry with a direct mercury analyzer (DMA-80), without prior sample treatment. Human health risk assessment was conducted using Estimated Weekly Intake (EWI), Target Hazard Quotient (THQ), and Maximum Safe Consumption Quantity (MSCQ) indices for both adults and children [1] (Table 1). Mean mercury concentrations ranged from 0.0338 to 0.1213 μg g^{-1}, with higher values observed in sarda and white croaker. None of the samples exceeded the maximum limit established by Brazilian legislation (0.5 μg g^{-1}). All calculated risk indices showed values below the established limits, according to the reference values of the USEPA [4] and FAO/WHO [2], indicating no risk to human health associated with the consumption of these species under the evaluated conditions. Despite the favorable results, continuous monitoring is recommended due to the increase in anthropogenic activities in the Amazon region.

Table 1. Fish species, mercury concentration, EWI, PTWI, THQ and MSCQ

Espécie	Hg (μg . g^{-1})	EWI (child)	EWI (adult)	PTWI % (child)	PTWI % (adult)	THQ (USEPA)	THQ (WHO)	MSCQ (USEPA) - Adult	MSCQ (USEPA) – Child	MSCQ (WHO) - Adult	MSCQ (WHO) – Child
Piramutaba (*Brachyplatystoma vaillantii*)	0,0338 ± 0,0072	0,1971	0,0845	12,31	5,28	0,0402	0,0524	621,30	266,27	476,33	204,14
Sarda (*Sarda sarda*)	0,1143 ± 0,0358	0,6667	0,2857	41,66	17,85	0,1360	0,1774	183,72	78,74	140,85	60,36
Pescada – Branca (*Plagioscion squamosissimus*)	0,1213 ± 0,0940	0,7075	0,3032	44,21	18,95	0,1444	0,1883	173,12	74,19	132,72	56,88

Table 1. Fish species, mercury concentration, EWI, PTWI, THQ and MSCQ.

Agradecimentos/Acknowledgments

The authors would like to thank CNPq and CAPES.

Determination of Water Content in bio-oil samples by Infrared Spectroscopy using portable and benchtop spectrometers: a comparative study

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Palavras Chave:*Thermal Liquefaction Bio-oil, IR, Water content.,Thermal Liquefaction, Bio-oil, IR, Water content*

Highlights

- Portable and benchtop IR spectrometers used for bio-oil quality control

- Predictive PLS models for water content have demonstrated satisfactory capability.

Resumo/Abstract

The growing need for decarbonization, driven by climate change, requires expanding the use of renewable energy sources to replace fossil fuels. In this context, the conversion of biomass into biofuels, such as bio-oil (a dark, viscous liquid used as a drop-in fuel precursor), can be a promising alternative for the energy transition. Thermal liquefaction (TL) stands out among the techniques used because it allows the use of water as a production solvent. This aligns TL with green chemistry principles. An important quality control parameter of bio-oils is the water content, as it affects properties, such as Higher Heating value (HHV). Although Karl Fischer titration (ASTM E203-24) is the reference method for water content determination, it has some disadvantages, such as being laborious, time-consuming, and requiring toxic and expensive reagents. Aiming to overcome these limitations, this work proposes alternative methods for water content determination in bio-oils produced by TL, using infrared spectroscopy (IR) and chemometrics. A total of 85 bio-oil samples were produced from different biomasses and production solvents, and their spectra were obtained using portable and benchtop instruments (around 70% for calibration, 30% for external prediction). Different pre-processing techniques were evaluated. Principal component analysis (PCA) revealed differences related to water content, especially for NIR spectrometers' data. The best models built using partial least squares (PLS) regression, for the range of 1-20% (w/w), demonstrated satisfactory and similar predictive capability: portable NIR-RMSEP = 1.61%; R^2 = 0.91; benchtop NIR-RMSEP = 1.85%; R^2 = 0.87, and benchtop MIR-RMSEP = 1.48%; R^2 = 0.90. There were no significant systematic errors at the 95% confidence level. Thus, IR spectroscopy associated with chemometrics proves to be an efficient tool for monitoring the water content of bio-oils.

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UFPE; LAC; FACEPE; CAPES; INCTAA

Determination of Zinc in Tampons: From Microwave Digestion to Digital Colorimetry via Smartphone

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Palavras Chave:*Digital Colorimetry,Zinc,Tampons,Green Chemistry,Sample Preparation*

Highlights

Eco-friendly Zn quantification in tampons using*smartphone*.

Resumo/Abstract

In recent years, colorimetry combined with digital image capture (DIC) has emerged as an important trend in analytical chemistry, driven by the demand for portable and green methods. This approach represents a strategic alternative for democratizing quality control of mass-consumption products, such as*tampons*, which are composed of cellulosic matrices and may act as vectors for accumulated metals [1,2]. In this context, zinc (Zn) determination is particularly relevant. Although essential, elevated Zn levels from agrochemical or industrial sources may cause cytotoxic effects in the vaginal mucosa, a highly vascularized and permeable tissue [3]. Notably, Brazilian regulation RDC No. 640/2022 does not establish limits for inorganic contaminants [4]. This work proposes a dual analytical approach. Initially, sample preparation was optimized by microwave-assisted digestion (MW-AD) of 500 mg of the sample using 3 mL of 30% (v/v) H_2O_2 and 7 mL of ultrapure water (10 min ramp to 200 °C and 30 min hold). Multielemental screening by FAAS enabled the quantification of Zn, Cu, Fe, and Mn, as well as the detection of trace amounts of Ni, Pb, Co, and Cr. For portable determination, a digital image analysis method based on the Zn(II)–PAN reaction was developed. Optimized conditions included 600 µL ammoniacal buffer (pH 9.5) and 120 µL PAN (250 mg L^{-1}). Images were acquired using a*smartphone*inside an MDF box equipped with 4000 K LEDs. Calibration curves were obtained by correlating Zn(II)–PAN concentrations with the ARGB analytical signal, showing linearity between 0.25 and 3.0 mg L^{-1}. The proposed method proved to be robust and effective for Zn determination in the analyzed samples.

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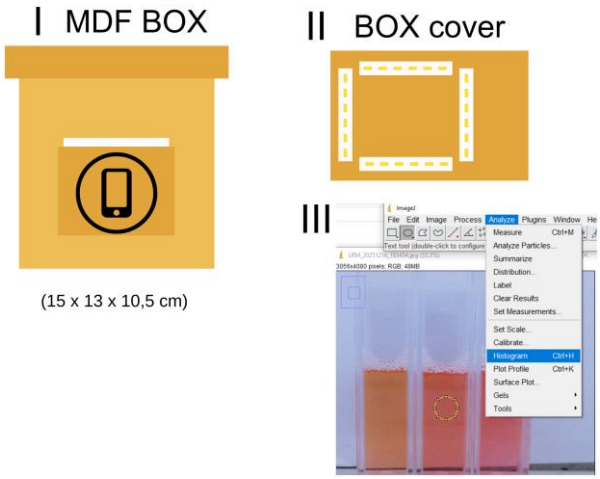


Fig.1: (I) MDF box for phone; (II) Lid w/ 4000K LEDs; (III) Color analysis & ROI in ImageJ.

Agradecimentos/Acknowledgments

The authors thank UFCAT for infrastructure. We acknowledge CNPq (scholarship), CAPES, FUNAPE and FAPEG for financial support, essential for this research.

Development and Aplication of an ultrasonic micronebulization system for determining contaminants in fuel ethanol by ICP OES.

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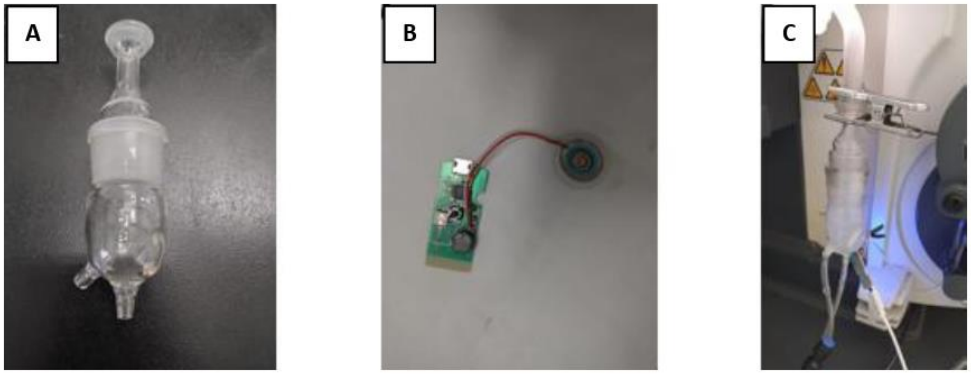
Palavras Chave:*ICP OES,nebulizers,fuels,inorganic contaminants,instrumental analysis*

Highlights

Development and evaluation of an ultrasonic nebulizer, Determination of metals in fuel ethanol, Improving analytical sensitivity and reduction of matrix effects.

Resumo/Abstract

The Brazilian National Agency of Petroleum, Natural Gas and Biofuels (ANP) classifies ethanol as a renewable biofuel, in contrast to other fossil fuels. However, the presence of inorganic contaminants in these fuels can cause severe problems in automotive engines, directly affecting their performance, being associated with human health issues, and contributing to environmental pollution. The determination of inorganic contaminants in fuels is challenging; nevertheless, the introduction of microsamples and ultrasonic nebulization are efficient strategies for trace-element determination by inductively coupled plasma optical emission spectrometry (ICP OES). This work developed a sample introduction system based on ultrasonic micronebulization ICP OES for inorganic contaminants in fuel ethanol. A piezoelectric transducer with a mesh of precise holes, ensuring uniform droplet size, was inserted into a lab-made spray chamber manufactured for this application. The radiofrequency power (W) and carrier gas flow rate (L min^{-1}) were optimized using a central composite design (CCD) with samples at different ethanol concentrations and the addition of 250 µL of V, Ni, Cu, Cd, Pb, As, Sb, and 5 mg L^{-1} of S. Additionally, HNO_3 0.43 mol L^{-1} and 5 mg L^{-1} Sc were used as internal standards. Optimal conditions were 52.5 % Ethanol; 1200.00 W; 0.6 L min^{-1}. Desirability plots showed no influence of ethanol on sensitivity. The Shapiro-Wilk test (α=0.05) verified normal distribution (p-value > 0.05). The calibration curve in HNO_3 0.21 mol L^{-1} showed sensitivity through the t-test, 95% confidence.The limits of detection (LOD) in mg L^{-1} for the HNO_3 curve were 0.02 for As, 0.02 for Cd, 0.19 for Cu, 5.08 for Ni, 21.91 for Pb, 0.16 for S, 0.2 for Sb and 0.06 for V. This system is efficient for fuel analysis.



Sistema de micronebulização ultrassônico

Agradecimentos/Acknowledgments

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Development and Validation of GC-FID and LC-MS/MS Methods for the Quantification of Major Cannabinoids in Commercial and Artisanal Cannabis Oils

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Palavras Chave:*Cannabis, Cannabinoids, Gas Chromatography, Validation*

Highlights

GC-FID and LC-MS/MS methods were developed and validated for cannabinoid quantification in commercial and artisanal cannabis oils, addressing degradation, derivatization, and matrix effects.

Resumo/Abstract

*Cannabis sativa*L. oils contain bioactive cannabinoids, mainly cannabidiol (CBD) and Δ⁹-tetrahydrocannabinol (THC), while cannabigerol (CBG) and cannabinol (CBN) also present pharmacological relevance. The growing demand for phytotherapeutic products has increased cannabis oil production; however, the high cost of commercial formulations has encouraged patient associations to produce artisanal oils, which often exhibit significant chemical variability. This scenario highlights the need for reliable, accessible, and standardized analytical methods. In this study, gas chromatography with flame ionization detection (GC-FID) and liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) methods are being developed and validated for cannabinoid quantification in commercial and artisanal cannabis oils. For GC-FID, chromatographic conditions were optimized, and an HP-5 column (30 m × 0.32 mm; 0.1 µm) provided efficient separation of the four target analytes with baseline resolution and a total run time of 15 min. The working range was established between 1 and 10 µg mL^{-1}, with good linearity (R^2 > 0.99) using standard addition calibration. Matrix effects were confirmed by statistically significant differences in calibration curve slopes. Thermal degradation was observed in non-derivatized standards, compromising quantitative accuracy. To mitigate this effect, samples were dried in a vacuum concentrator and derivatized by silylation using BSTFA:TMCS with pyridine at 60 °C for 15 min, showing adequate robustness. Sample clean-up by C18 solid-phase extraction or liquid-liquid extraction is under evaluation to minimize matrix effects. The LC-MS/MS method is under development using a C18 column, with optimization of mass transitions and mobile phase. Both methods will be fully validated according to ANVISA RDC 166/2017.

Agradecimentos/Acknowledgments

We would like to thank the financial support from CNPq, FAPESP, CAPES, FINEP, and FAEPEX-UNICAMP.

Development of a dual fluorimetric-spectrophotometric method for protein determination using probe-based approaches

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Palavras Chave:*Probe,Hemoglobin,dual method,biotechnological applications*

Highlights

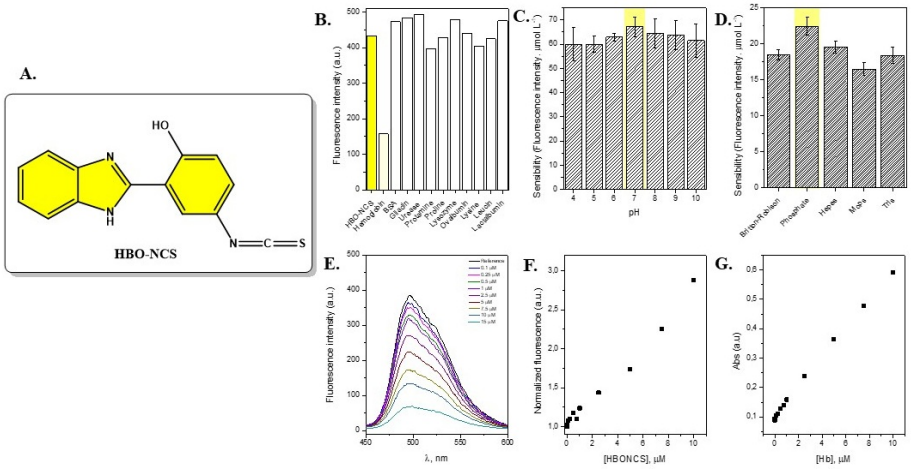
A dual fluorimetric-spectrophotometric method using HBO-NCS was developed for sensitive hemoglobin determination, with LOD 0.38 µM, LOQ 1.27 µM, and RSD 2.3–2.9%.

Resumo/Abstract

Proteins are biomolecules that are crucial for biological processes, performing structural, catalytic, and transport functions [1]. Hemoglobin (Hb), in particular, is an important marker in clinical and forensic analyses. Therefore, the development of methods for its determination is essential, as it allows for more sensitive, accurate, and efficient analyses, in addition to expanding the possibilities for application and reliability of results [1,2]. Thus, in this study, a benzazole isothiocyanate derivative (HBO-NCS) (Fig. 1A) was explored as a dual method (fluorimetric-spectrophotometric) for determining Hb. Using analytical sensitivity as an evaluation criterion, the following results were obtained: the HBO-NCS probe was selective for Hb (Fig. 1B); pH 7.0 showed the highest sensitivity for evaluating the HBO-NCS-Hb system (Fig. 1C); phosphate buffer showed the highest sensitivity (Fig. 1D); at a concentration of 20 mM, which was chosen for further studies; under optimized conditions, the method presented LOD = 0.38 µM, LOQ = 1.27 µM, linear range = 0.1–10 µM (Fig. 1E–G), and RSD between 2.3–2.9%; Finally, the dual method developed proved to be simple and selective and can be used for the determination of Hb in real samples.

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HBO-NCS probe and results obtained in studies against Hb

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Development of a molecularly imprinted monolithic coating for sorptive and selective stir bar extraction of acetamipride in liquid samples

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Palavras Chave:*Sample preparation, neonicotinoids, sorbent microextraction, separation methods,Sample preparation, Neonicotinoids, Sorbent Microextraction, Separation methods*

Highlights

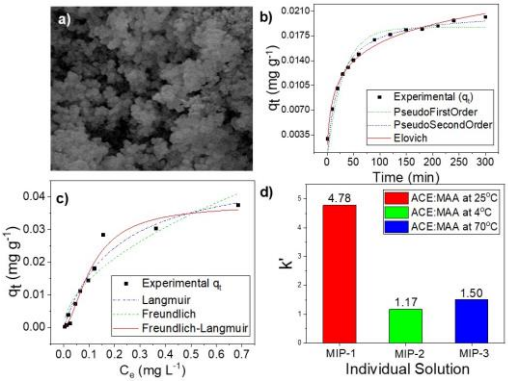
Development of a molecularly imprinted monolithic coating for SBSE

Selective coating for acetamiprid in the presence of imidacloprid

Covalent molecular imprinting between acetamiprid and MAA

Resumo/Abstract

Currently, the low selectivity of commercial coatings (PDMS, PEG, and PA) used in stir bar sorptive extraction (SBSE) limits the applicability of this technique. In this context, the use of molecularly imprinted (MIP) methacrylate-based polymer monoliths is a promising alternative, enabling the formation of specific molecular recognition sites and expanding the technique's applicability. In this work, a selective SBSE monolithic MIP coating for acetamiprid (ACE) was developed for determining this pesticide residue in food samples. The sorptive coating synthesis consisted of the*in situ*copolymerization of trimethylolpropane triacrylate, methacrylic acid (MAA), ethylene glycol dimethacrylate, and 2,2'-azobisisobutyronitrile with 70% toluene. Non-imprinted coatings (NIP-SBSE) were polymerized with 250 µL of monomeric solution using a 2.5×6 mm magnet (60 °C, 1 h, argon). Molecularly imprinted coatings (MIP-SBSE) were prepared from the prior complexation of ACE:MAA at different temperatures (4, 25, 70 °C, 1h), followed by polymerization at 60 °C and cleaning (MeOH). The SBSE tests were performed under stirring at 25 rpm and 25 °C, and the NIP-SBSE were evaluated for kinetics and for the acetamiprid adsorption isotherm by high-performance liquid chromatography with a diode-array detector. Scanning electron microscopy (SEM) and N_2 adsorption characterizations indicated a highly porous material with a surface area of 77 m²/g. Adsorption studies indicated a maximum adsorption capacity (q_{max}) of 0.03 mg/g, fitting the Langmuir-Freundlich model (R^2 = 0.97), while the kinetics followed the Elovich model (R^2 = 0.98). The relative selectivity (k') of MIP-SBSE, related to a structural analog of imidacloprid (IMI), showed values > 1, evidencing specific interactions of the MIP coating and acetamiprid. Selectivity studies in binary solutions consisting of similar structures (ACE and IMI) and the application of MIP-SBSE in the extraction of ACE from liquid food samples are ongoing.



a) SEM, b) adsorption kinetics, c) NIP adsorption isotherm, and d) relative selectivity of MIP

Agradecimentos/Acknowledgments

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DEVELOPMENT OF A SUSTAINABLE AND COST-EFFECTIVE SMARTPHONE-BASED DIGITAL IMAGE METHOD TO DETERMINE POTASSIUM BROMATE IN BREADS

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Palavras Chave:*Bakery products,Food Safety,KBrO3,RGB,Smartphone*

Highlights

Smartphone-based method to monitor $KBrO_3$ in commercial breads;

Fast and portable analytical tool for food quality control;

Ten samples of bread tested positive for the prohibited $KBrO_3$.

Resumo/Abstract

Potassium bromate is a commonly used additive as a flour improver in baked goods; however, its use is prohibited in Brazil (National Health Surveillance Agency - ANVISA, Law No. 10.273/2001)[1] due to its potential carcinogenic and genotoxic effects, making its quantification necessary for food safety purposes. We aimed to develop a green analytical method for the identification and quantification of potassium bromate in breads using smartphones, based on direct digital image acquisition (DIA). The proposed method presents itself as an accessible and efficient alternative compared to the reference method using molecular absorption spectrophotometry by UV-Vis spectrometer. We have used Color Grab® and REDGIM®free software, and DIA was applied to construct the analytical curves focusing on the RGB and HSV color channels in the concentration range from 0.25 to 10 μg mL^{-1}, resulting in high linearity, evidenced by correlation coefficients (R^2) greater than 0.99, LOD of 0.14 μg mL^{-1}, and LOQ of 0.42 μg mL^{-1}. Twenty-two commercial bread samples made from wheat flour were obtained from the Metropolitan Region of Recife (RMR), Pernambuco state (Brazil). The results were also statistically similar to the UV-Vis reference method. The concentrations detected by the DIA method ranged from 3.19 to 23.02 μg g^{-1} in ten samples of commercial breads. Recovery percentages ranged from 90.94% to 105.65%, meeting the criteria established by international guidelines for analytical methods (INMETRO, 2003). Evaluated using the Modified Green Analytical Procedure Index (MoGAPI), the method showed considerable advantages over the UV-Vis reference method. The smartphone-based digital image method allows for in situ applications and promotes continuous monitoring of food quality, contributing significantly to food inspection in line with Green Analytical Chemistry (GAC), with potential for implementation in bread quality control.

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Agradecimentos/Acknowledgments

CAPES, CNPq, FACEPE, LaMTESA, PEM Research Group

Development of a Total Suspended Particles (TSP) Sampler and Elemental Determination by ICP-OES

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Palavras Chave:*Atmospheric pollution; Particulate matter; Acid extraction; Potentially toxic metals; Spectrometry.*

Highlights

Development of a low-cost TSP sampler using alternative materials for air quality monitoring. Gravimetric determination of TSP concentration and multielemental analysis by ICP-OES.

Resumo/Abstract

Total Suspended Particles (TSP) are microscopic particles dispersed in the air that vary in and chemical composition. They are classified as atmospheric pollutants and, depending on their concentration and composition, may cause adverse effects on human health and the environment. In this context, the aim of this study was to develop a low-cost TSP sampler to determine the concentration of this pollutant and evaluate its chemical composition. The sampler was constructed using an air suction pump and alternative materials and was applied to collect samples at five sites in the municipality of Itapetinga, Brazil. The system operated at a flow rate of 16.7 L min^{-1} for 48 hours, and TSP samples were collected on fiberglass filters. Particle mass was determined by gravimetric analysis. Considering the sampled air volume, TSP concentrations ranged from 16.63 to 41.37 µg m^{-3}, values below the maximum limits established by Brazilian legislation.
For elemental analysis, the samples were digested using HNO_3, HCl, and H_2O_2 in a digestion block at 180 °C for 2 hours. The concentrations of As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, S, Sb, Sr, V, and Zn were determined by ICP-OES. Method accuracy was evaluated using certified reference materials (BCR-176R and NIST 1648a). The method presented satisfactory precision and low detection limits for the analyzed elements. Concentrations in the samples (ng m^{-3}) ranged from 4.1 – 11.2 (As), 2.9 – 4.4 (Cd), 1.1 – 3.2 (Co), 11.9 – 18.5 (Cu), 408 – 1439 (Fe), 11.8 – 26.0 (Mn), 1.5 – 7.3 (Ni), 4.7 – 14.4 (Pb), 232 – 418 (S), 2.2 – 10.7 (Sb), 25.6 – 70.4 (Sr), 1.01 – 1.70 (V), and 790 – 6516 (Zn). Arsenic concentrations exceeded the limits established by the European Union, while Brazilian legislation does not define a maximum level for this element in ambient air. For the other elements, concentrations remained below the regulatory limits considered in this study.



Figure 1. TSP collected on fiberglass filter

Agradecimentos/Acknowledgments

Agradecemos aos membros da equipe de pesquisa pela colaboração, à UESB pelo apoio institucional e às agências de fomento pelo suporte essencial concedido a este estudo

Development of Machine Learning Models for the Classification of New Psychoactive Substances (NPS) via Mass Spectrometry

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Palavras Chave:*New Psychoactive Substances (NPS), Mass Spectrometry, Machine Learning, Forensic Chemistry, LightGBM,New Psychoactive Substances (NPS),,Mass Spectrometry,New Psychoactive Substances (NPS),Machine Learning,Forensic Chemistry,LightGBM*

Highlights

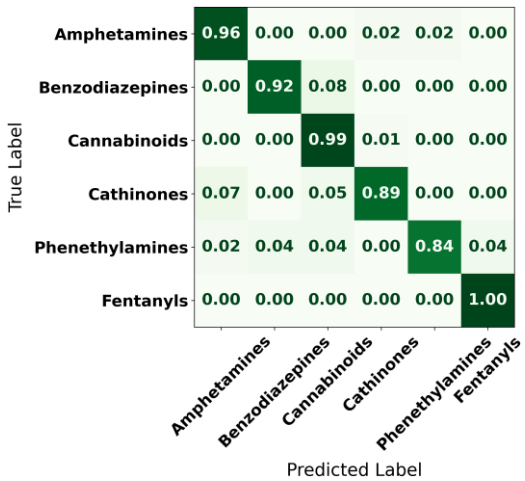
AI-driven classification of New Psychoactive Substances using LightGBM achieves a 94% F1-score, optimizing forensic analysis and public safety strategies.

Resumo/Abstract

The rapid emergence of New Psychoactive Substances (NPS) poses a critical challenge to forensic science, given the structural diversity and the frequent lack of analytical reference standards. According to SWGDRUG, mass spectrometry (MS) is a category A technique, essential due to its high structural selectivity. This work proposes the development of a machine learning model for the automated classification of NPS from MS data, aiming to fill information gaps and assist in the analyst's decision making.

The dataset was composed of 1,337 spectra obtained from the SWGDRUG library, distributed into six classes: cannabinoids, fentanyls, amphetamines, phenethylamines, cathinones, and benzodiazepines. The raw intensities from*m/z*1 to 690 were used as predictor variables (features), without applying preprocessing, aiming for analytical workflow efficiency. The initial algorithm screening was performed using PyCaret library, followed by hyperparameter optimization via Scikit-learn. The final model was validated using 10-fold stratified cross-validation.

The LightGBM (LGBM) algorithm showed superior performance, achieving a global accuracy of 0.95 and a macro F1-score of 0.94. Notably, the performance within the fentanyl class stands out with an F1-score of 0.99, highlighting the model robustness for substances of high toxicological criticality. The confusion matrix analysis revealed efficient segregation between amphetamines and cathinones, despite their structural homology (β-keto- phenethylamines). The phenethylamine class showed the highest error dispersion (Recall 0.84), reflecting its intrinsic spectral variability. The proposed methodology demonstrates technical viability as a strategic screening tool, with direct implications for public safety policies and harm reduction.



Normalized confusion matrix (LightGBM) for NPS classification using 1,337 MS spectra.

Agradecimentos/Acknowledgments

Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, PIBIC e INCT-SP: 406958/2022-0. Coordenação para o Aperfeiçoamento de Pessoal de Nível Superior: (CAPES, Financial Code 001)

Development of Sample Preparation and Chromatographic Separation for the Enantioselective Analysis of the Pesticide Cyflumetofen in Liver Microsomes

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Palavras Chave:*Cyflumetofen,Enantioselective separation,Chiral liquid chromatography,Experimental design,Full factorial design*

Highlights

Multimodal LC screening with polysaccharide-based columns.

Chiralcel OJ-R stood out as the best CSP for cyflumetofen enantioseparation.

Resumo/Abstract

Cyflumetofen (CIF) is a chiral acaricide whose environmental and biological behavior is influenced by its stereochemistry. Its chirality can lead to significant differences in efficacy against target organisms and toxicity toward non-target species. Since CIF residues have been detected in food matrices, developing enantioselective analytical methods is imperative for monitoring human exposure and ensuring accurate toxicological risk assessments by distinguishing individual enantiomers. The analytical strategy involved a chromatographic screening of ten polysaccharide-based chiral columns, evaluating reversed-phase and polar organic modes. Analyses were conducted at 30 °C with a 20 µL injection volume and the flow rates varied between were 0.5 mL/min and 0.3 mL/min. Chiral separation was assessed by resolution and peak symmetry, identifying the Chiralpak OJ-R column (150 × 4.6 mm, 5 µm) as the most efficient. The optimized condition used reversed-phase mode with methanol:water (80:20), resulting in a 15-min run time. Under these conditions, resolution was higher than 1.5. Subsequently, as our aim is to analyze this pesticide in a biological matrix, sample preparation was optimized via a full factorial design using liver microsomes as sample matrix. The optimal condition consisted of the liquid-liquid extraction using 500 µL of ethyl acetate. The protocol involved agitation (500 rpm) for 20 min followed by centrifugation at 1600 xg for 10 min. According to the experimental design, the time and speed of agitation were the only factors with statistical significance ($p \leq 0.05$) on extraction efficiency, while the solvent volume did not exert a decisive influence. Under this condition the mean recovery was 88% with RSD values below 5%. In addition, no interferences were detected in the retention times of the target analytes. The integrated method demonstrated robustness and efficiency for future toxicological investigations.

Agradecimentos/Acknowledgments

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DGT-type devices for the determination of atrazine, ametryn, and diuron in aqueous matrices using cork as the binding phase

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Palavras Chave:*Passive sampling,Alternatives sorbents,Experimental design,Method developments*

Highlights

DGT method with cork discs for ATZ, DIU and AMT in water.

Sorption up to 59% and recoveries 86–108%.

Desorption optimized by 2^2 factorial design.

Cork proved suitable for low-cost monitoring.

Resumo/Abstract

Pesticides, especially herbicides, although essential for agricultural productivity, pose environmental and public health concerns due to their indiscriminate use, highlighting the need for sensitive, effective and preferably low-cost analytical methods for their determination in aqueous matrices. In this context, passive sampling using diffusive gradients in thin films (DGT) has emerged as promising alternative. DGT devices consist of a diffusive layer that controls analyte transport and a binding phase responsible for retention, followed by analyte elution and quantification. This study aimed to develop and optimize a DGT-based analytical protocol using cork discs as an alternative binding phase for the determination of atrazine (ATZ), diuron (DIU), and ametryn (AMT) in aqueous matrices. Cork sorption capacity was evaluated in 24 h sorption experiments, yielding retention values of 31 ± 1 % for ATZ, 47 ± 3 % for DIU, and 59 ± 9 % for AMT. Desorption conditions were optimized using ultrasound-assisted organic solvent mixtures through a 2^2 factorial design. Optimal conditions were achieved with a 25:75 methanol/acetonitrile mixture and 5 min of sonication, resulting in recoveries of 86 % for ATZ, 108 % for DIU, and 97 % for AMT. The diffusive layer consisted of a 1.5% (m/v) agarose gel with a thickness of 0.8 mm. Apparent diffusion coefficients determined over one week were 1.43×10^{-6}, 4.21×10^{-7} and 4.21×10^{-6} cm² s^{-1} for ATZ, DIU and AMT, respectively. Overall, the results demonstrate that cork provides adequate performance as a DGT binding phase, confirming the applicability of this approach for environmental monitoring in aqueous systems.



DGT device with cork as the binding phase and 1.5% agarose gel as the diffusive phase

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Dye–polymer interactions by UV–Vis: effects of pH, matrix composition, concentration and salinity

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Palavras Chave:*Polymers,Produced water,Cationic dyes,UV–Vis spectrophotometry*

Highlights

Cationic dye–polymer interactions enable UV–Vis detection of anionic polymers in produced water; matrix, pH and concentration drive band shifts/hypochromic effects via electrostatic & π–π interactions

Resumo/Abstract

Monitoring polymers in saline wastewater is essential to reduce operational impacts, evaluate reuse potential, and ensure environmentally sound disposal. The reference method of these polymers determination is size exclusion chromatography (SEC) with UV or IR detection; however, its complexity limits on-site application, motivating the search for simpler analytical alternatives.

This study investigates the use of cationic dyes for detecting high molecular weight anionic polymers in saline matrices by UV–Vis spectrophotometry. Toluidine blue, basic fuchsin, and methylene blue were used as dyes, and a sulfonated high molecular weight polymer commonly used in industrial applications was evaluated. Spectral results showed that matrix composition, pH and polymer concentration strongly affect dye–polymer interactions, producing band shifts and absorbance changes. At acidic and neutral pH, toluidine blue exhibits a band at 632 nm (monomeric form), methylene blue at 665 nm and basic fuchsin at 545 nm. Upon polymer addition to the aqueous medium, bands exhibit a hypochromic effect, with decreasing intensity at higher polymer concentrations, accompanied by the emergence of new bands at 562 nm (toluidine blue), 590 nm (methylene blue) and 486 nm (basic fuchsin). These effects are attributed to electrostatic interactions and π–π interactions resulting from aggregation of the aromatic rings present in the dyes.

High ionic strength suppressed these effects because dissolved ions competed with polymer groups, reducing dye affinity and resulting in minimal spectral variation. Dialysis reduced salinity, resulting in an effect similar to that observed in aqueous solutions, and allowing significant spectral variations that confirmed polymer presence, enabling clear polymer detection. The methodology proposed based on the polymer-dye interactions demonstrated high potential for polymer detection, with dialysis improving applicability in saline wastewater.

Agradecimentos/Acknowledgments

This study was supported by PUC-Rio, PRIO and Human Resources Training Program of the Brazilian National Agency for Petroleum, Natural Gas and Biofuels (PRH-ANP). A.P.G. thanks support from FAPERJ (204.241/2024) and CNPq (310713/2025-0).

Efeito do enriquecimento de cebolinha (Allium schoenoprasum L.) com selênio na distribuição de elementos essenciais

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Palavras Chave:*selênio,cebolinha,enriquecimento,elementos essenciais*

Highlights

Chives are easy to grow and popular in Brazil. Hydroponics offers advantages for elemental enrichment, but its success depends on effects on the translocation and accumulation of essential elements.

Resumo/Abstract

Hortaliças integram boa parte da alimentação da população brasileira, destacando a cebolinha*Allium schoenoprasum L.*, que é de fácil cultivo, inclusive o hidropônico, e amplamente utilizada como condimento no Brasil. É possível destacar que a hidroponia agrega vantagens como uma promissora alternativa de enriquecimento elementar. É fundamental destacar a necessidade de se conhecer as espécies elementares capazes de serem absorvidas, utilizadas pelas plantas no seu metabolismo e acumuladas nas partes comestíveis, bem como as espécies formadas após o enriquecimento, sendo necessário avaliar se esses alimentos fortificados apresentam as mesmas características químicas daquelas formadas quando o alimento é cultivado em condições naturais do solo e livre de metais tóxicos. Assim sendo, para o sucesso do enriquecimento, é fundamental avaliar o seu efeito na translocação e acúmulo de elementos essenciais. Desta forma, neste trabalho avaliou o efeito do cultivo hidropônico de cebolinha utilizando meio enriquecido com Se na distribuição de elementos essenciais (Ca, Cu, Fe, P, S, Se e Zn) por ICP OES. As condições de cultivo foram estudadas e soluções de 5, 10 e 50 mg L^{-1} Se(VI) foram aplicadas para o enriquecimento. Após 14 dias, as folhas foram cortadas, secas e moídas. Para a análise por ICP OES, as amostras serão submetidas à digestão com mistura oxidante diluída e aquecimento em forno de micro-ondas. Teste de adição e recuperação será feito para verificar a existência de interferências químicas. Comparações com o grupo controle (não enriquecido) serão feitas para verificar o efeito do enriquecimento na distribuição dos elementos essenciais.

Agradecimentos/Acknowledgments

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Electrochemical sensing platform based on BiVO 4 /graphene oxide/MIP-iniferter electrode for 1-(3-chlorophenyl)piperazine illicit drugdetermination

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Palavras Chave:*Electroanalysis; MIP-sensor; Non-enzymatic sensor*

Highlights

A novel mCPP sensor was developed using a hybrid $BiVO_4$/GO/MIP material.
Sinergic effect of $BiVO_4$and graphene oxide/MIP was observed.
Highly selective mCPP determination was noticed.

Resumo/Abstract

1-(3-chlorophenyl)piperazine (mCPP) is a psychoactive substance with high hallucinogenic and stimulant effects, with increasingly recreational purposes worldwide. Its growing occurrence in illicit formulations, together with the limited availability of accessible and rapid monitoring strategies, highlights the demand for sensitive and selective detection methods. Herein, we report a simple, fast, and selective electrochemical approach for mCPP determination in seized samples. The sensor is based on a hybrid material comprising monoclinic $BiVO_4$ and an imprinted poly(methacrylic acid) grafted onto iniferter-modified graphene oxide (GO/MIP) through living-radical polymerization (BVO:GO/MIP). A physical mixture of the materials was drop-cast onto a fluorine-doped tin oxide (FTO) electrode. Sensor design and experimental conditions were optimized and evaluated using cyclic voltammetry, chronoamperometry, and electrochemical impedance spectroscopy. mCPP exhibited an irreversible oxidation peak at +0.90 V vs. Ag/AgCl on the BVO:GO/MIP electrode in 0.3 mol L−1 HEPES buffer (pH 7.00) as the electrolyte solution. Under optimized conditions, amperograms showed a linear response and satisfactory R^2 of 0.99942 over 2.33–220 µmol L−1, with a limit of detection = 0.7 µmol L^{-1} calculated as 3σ/slope, where σ represents the standard deviation of 10 measurements of the blank. Absence of signals was observed from some adulterants and other classes of drugs of abuse found in seized samples, including lidocaine, acetaminophen, acetylsalicylic acid, caffeine, benzocaine, procaine, phenacetin, methamphetamine, methylone, and mephedrone. The method was applied to a spiked ecstasy sample, and accuracy was confirmed by comparison with HPLC-DAD as the reference method. Overall, the developed method shows strong potential as a rapid, selective, low-cost, and straightforward screening tool for mCPP in forensic samples, with reduced environmental impact according to the AGREE score (0.75).

Agradecimentos/Acknowledgments

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Environmentally friendly extraction of acrylamide and 5-hydroxymethylfurfural from coconut water samples using DPX

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Palavras Chave:*Green analytical chemistry,coconut water samples,acrylamide and HMF,high-performance liquid chromatography with ultraviolet detector,disposable pipette extraction.*

Highlights

Microextraction enabled the same sorbent to be reused 72 times for extracting acrylamide and HMF from coconut water samples

Resumo/Abstract

This work aimed to develop a methodology for the extraction using Disposable Pipette Extraction (DPX) and determination by High-Performance Liquid Chromatography with an Ultraviolet detector of acrylamide (AC) and hydroxymethylfurfural (HMF) in coconut water. The chromatographic method was developed using the MZ Aqua Perfect C18 column with isocratic elution in 5.00% (v/v) acetic acid, a flow rate of 0.60 mL/min, and a wavelength of 210 nm, enabling the detection of AC and HMF with retention times of 6.06 and 13.80 min, respectively. DPX was prepared using 1.0 mL micropipette tips with silica-based sorbent and a hydrophilic polypropylene frit at the bottom of the SPE cartridge. The sorbent type and mass (silica bonded with octadecyl (C18) or octyl (C8)), the conditioning solvent type and volume (methanol and SDS solutions), and eluent volume were optimized to improve extraction efficiency. The optimized parameters included using 600 mg C18 as support with conditioning (325 µL of 0.05 mol/L SDS with 7.50% isopropanol and pH 3.00 buffer), a sample volume of 1000 µL, and elution with 775 µL methanol, achieving about 90% recovery for both analytes. Analytical curves were built with a linear range of 50.0-750 µmol/L for AC and of 5.00-100 µmol/L for HMF, along with quantification (0.13 and 0.06 µmol/L for AC and HMF, respectively) and detection (0.04 and 0.02 µmol/L for AC and HMF, respectively) limits, repeatability (4.04 and 3.51% for AC and HMF, respectively). This method was used on pasteurized coconut samples, with recovery values from 85.36% to 107.04%. The greenness was assessed using ComplexMoGAPI (84), BAGI (77.5), and AGREEprep (0.69), enabling 72 reuses for extracting AC and HMF, with recovery rates from 94.72% 98.32%. The proposed method for extracting AC and HMF offers several benefits, including using less sorbent, solvent, and sample, being fast and inexpensive, and not requiring a vacuum system, and aligning with Green Analytical Chemistry principles.

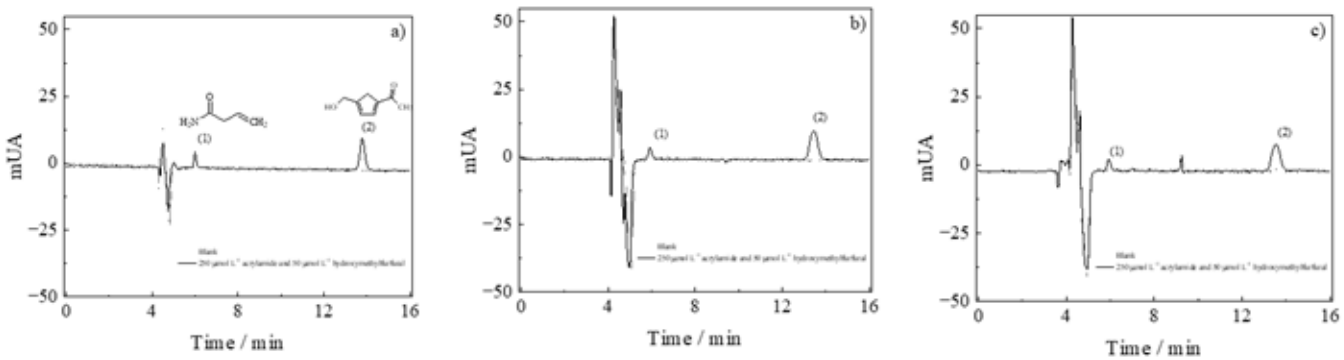


Fig 1: Chromatograms of 250 µM AA and 25 µM HMF in: a) water, b) DPX (MeOH), c) DPX (coconut water).

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CAPES (001), CNPq (305538/2022-5), and FAPESP

Espectroscopia NIR como ferramenta auxiliar na seleção preliminar de genótipos com perfil alto oleico em programas de melhoramento de soja.

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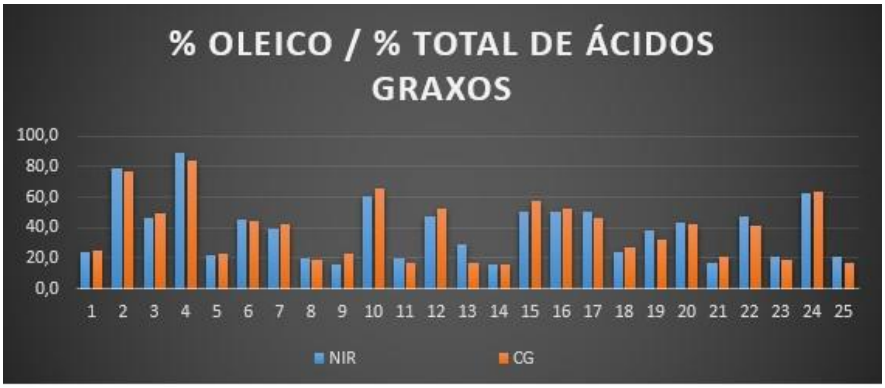
Palavras Chave:*NIR, Alto Oleico, Ácidos graxos, Melhoramento, Soja,NIR,Alto Oleico,Ácidos graxos,Melhoramento,Soja*

Highlights

High-oleic soybean breeding accelerated by NIR spectroscopy as GC alternative. Model performance: R^2=0.994, SEP=1.39. Low-cost, dynamic screening of genotypes high-oleic soybean selection programs.

Resumo/Abstract

A seleção de genótipos de soja com perfil alto oleico é essencial para acelerar o desenvolvimento de cultivares que aliem desempenho agronômico e qualidade de óleo. Este trabalho propõe o uso da espectroscopia NIR como alternativa rápida e sustentável à cromatografia gasosa na seleção preliminar em programas de melhoramento. Foram selecionadas 190 amostras de linhagens e cultivares de soja com perfil variado de ácidos graxos, e a coleta dos espectros dos grãos para desenvolvimento dos modelos preditivos foi realizada em espectrômetro FT NIR Antaris II, operando de 1100 a 2500 nm em refletância difusa, resolução de 4 cm^{-1} e média de 32 scans por coleta. Em seguida, as amostras foram moídas e tiveram seus teores de ácido oleico determinados por cromatografia gasosa em triplicata, seguindo metodologias oficiais descritas por ABIDI*et al.*(1999), BANNON*et al.*(1982), CHRISTIE (1989) e RAYFORD*et al.*(1994). Os dados foram modelados por PLS e explorados por PCA, com validação cruzada e conjuntos independentes para avaliação da robustez. As regiões de 1160-1180, 1400-1420 e 2140-2180 nm destacaram-se como mais informativas para predição do ácido oleico, por estarem associadas às vibrações C–H dos ácidos graxos, em concordância com estudos prévios sobre óleos vegetais. O modelo desenvolvido especificamente para predição do ácido oleico em soja apresentou coeficiente de determinação (R^2) 0,99431 e erro padrão de predição (SEP) de 1,39. A validação externa com sementes individualizadas de 25 linhagens promissoras não apresentou diferença significativa entre os métodos. Os dados comprovam o sucesso do melhoramento genético na alteração do perfil lipídico da soja e incremento da proporção de ácido oleico, e a espectroscopia NIR surge como ferramenta interessante para a seleção de linhagens de forma dinâmica e com baixo custo analítico, reduzindo o tempo necessário para o avanço de geração até a obtenção de uma cultivar comercial com o perfil alto oleico estabelecido.



Validação externa de modelo de predição NIR para teor de ácido oleico em grãos de soja

Agradecimentos/Acknowledgments

Agradeço a Deus, aos meus familiares e colegas de trabalho pelo apoio, ao programa de Melhoramento em Soja da Embrapa pelo suporte na condução das análises, e ao Programa de Pós-Graduação em Química da Universidade Estadual de Londrina.

Evaluation of Acid Decomposition in a Closed Block Using a 2^3 Design for Multielement Analysis of Oilseed Flours by ICP OES

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Palavras Chave:*Nutritious flours,acid decomposition,ICP OES,Multivariate analysis,Green Analytical Chemistry,Acid decomposition*

Highlights

An eco-friendly method for multi-element analysis in oilseed flours by ICP OES.
A full factorial design 2^3 was employed for dilluted nitric acid decomposition procedure optimization.

Resumo/Abstract

Oilseed flours are promising functional ingredients due to their high levels of bioactive compounds and nutrients; however, the complex matrix rich in lipids and fibers requires efficient sample preparation for elemental analysis. In this study, an acid decomposition method in a closed digestion block was developed as an alternative to microwave-assisted digestion (MWAD). The variables nitric acid concentration (3.0–7.0 mol L^{-1}), time (60–120 min), and temperature (160–180 °C) were evaluated using a full 2^3 factorial design, while sample mass (250 mg), addition of 1 mL of H_2O_2 (30% m m^{-1}), and a final volume of 5 mL were kept constant. The normalized multi- response, based on spectrometric analytical signals, was used in the experimental design. The Pareto chart showed no significant effects of the studied variables, indicating that gentler conditions are enough to achieve proper matrix digestion. Therefore, the minimum levels were chosen for all tested variables (3.0 mol L^{-1} HNO_3 at 160 °C for 60 min), as using lower reagent amounts, shorter heating durations, and lower temperatures reduces input use, chemical waste, and energy consumption, aligning with Green Analytical Chemistry principles. The analytical method showed precision (RSD < 3%) and accuracy with recoveries ranging from 94% to 110% compared to the reference MWAD method. Limits of quantification ranged from 0.1 to 34.3 mg kg^{-1}. Nine elements (Cu, Fe, Mn, Ni, Zn, Ca, K, P, and Mg) were determined in 32 samples of coconut, almond, peanut, and flaxseed oilseed flours. Application of PCA and HCA identified three main clusters and similarity between samples, showing that while coconut and peanut flours formed distinct groups, almond samples were distributed between the flaxseed and peanut clusters due to shared mineral characteristics. The proposed method proved to be eco-friendly and cost-effective, enabling simultaneous digestion of oilseed flour samples with analytical performance comparable to MWAD.

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Evaluation of Different Normalization Strategies for Cellular Metabolomics Data

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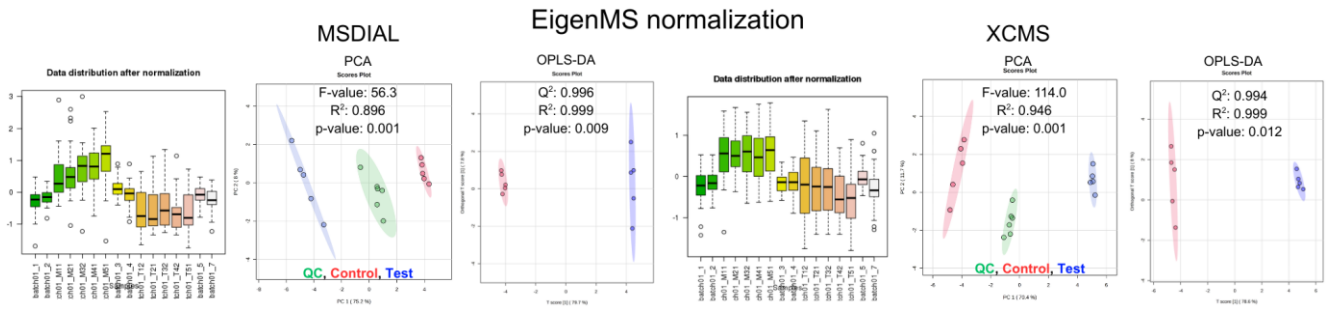
Palavras Chave:*normalization strategies,untargeted metabolomics,GC-MS,chemometrics*

Highlights

Nine normalization strategies were evaluated on metabolomic data obtained by GC-MS, processed by two freely available software. Based on different criteria, EigenMS algorithm had the best performance.

Resumo/Abstract

Untargeted metabolomics is the comprehensive study of all metabolites in a biological organism to understand their relevant biological variations. Therefore, unwanted variations arising during sample preparation and data acquisition must not interfere with the biological response of interest. To overcome these issues, normalization steps are performed during data processing, becoming a fundamental step in the workflow. Different normalization strategies are available, and there is no consensus on the best strategy. Thus, this study aimed to compare nine post-acquisition normalization strategies (contrast, EigenMS, linear baseline, Mass Spectrometry Total Useful Signal (MSTUS), mean, median, Probabilistic Quotient Normalization (PQN), quantile, and total-sum) in a cellular metabolomics dataset acquired by gas chromatography-mass spectrometry (GC-MS). The data were processed using two freely available software (MS-DIAL and XCMS). Normalization strategies were applied in the NOREVA platform. The results were evaluated by unsupervised multivariate models (principal component analysis) and data distribution (loadings plot and within-group relative log abundance). For both processing software, EigenMS was defined as the best normalization approach. This strategy showed the best sample grouping, with significant models (p-value = 0.001) and R2> 0.9. A proper and homogeneous data distribution was also observed (Figure 1). Although EigenMS has demonstrated superiority in normalizing these cellular data, it is important to emphasize that there is no universally applicable normalization strategy. Therefore, a careful evaluation of different normalization methods is recommended for each specific set of metabolomic data.



EigenMS normalization results (data distribution, PCA, and OPLS-DA) for both software.

Agradecimentos/Acknowledgments

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Evaluation of potentially toxic metal availability in electronic cigarette foams

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Palavras Chave:*E-cigarrets, toxic metallic ions, FAAS*

Highlights

Metal ions were detected in foams from used e-cigarettes; Acid extraction enhanced metal ion availability; Foams may act as a source of toxic metals to the environment

Resumo/Abstract

The increasing popularization of electronic cigarettes has raised public health concerns due to the toxicity of the substances present in these devices. However, the environmental impact associated with the improper disposal of these products also deserves attention, considering their high consumption and the consequent generation of waste. Given the presence of metallic components in the structure of e-cigarettes, this study investigated the release and availability of metallic ions present in the foams of used devices. Foams obtained from e-cigarettes of 11 different brands, containing flavoring liquids with distinct aromas, were analyzed. The ions Ni, Co, Cu, Zn, Mn, Fe, Cr, and Pb were evaluated. Samples (0.05 g) were subjected to extraction using two eluents: deionized water (10 mL) and 0.1 mol L^{-1} nitric acid (10 mL). The samples were placed in an ultrasonic bath for 30 minutes, and after foam removal, the extracts were analyzed by flame atomic absorption spectroscopy (FAAS). Although most FAAS signals indicated concentrations below the quantification limit of the technique, the ions Ni, Co, Cu, Zn, and Mn were detected after extraction with nitric acid. In aqueous extraction, the ions Cu, Zn, Mn, and Pb were detected. Energy-dispersive X-ray spectroscopy (EDX) was employed as a complementary technique for qualitative confirmation, with direct analysis of the foams without prior extraction. The presence of all evaluated ions was confirmed, corroborating the results obtained by FAAS. Manganese was detected in 100% of the analyzed samples, while copper and cobalt were present in 54.5% and 36.4% of the samples, respectively. Nickel and zinc showed lower detection frequencies, at 27.3% and 9.1%, respectively. It can be concluded that, although the release of metallic ions in aqueous media is limited, the composition of the foams may act as a potential source of toxic substances, posing risks to both user health and the environment.

Agradecimentos/Acknowledgments

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Evaluation of RP-DLLME for further alkaline and alkaline-earth metals determination in crude oil atmospheric and vacuum residues by ICP-OES

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Palavras Chave:*RP-DLLME; Crude oil AR, Crude oil VR, alkaline and alkaline-earth metals ICP-OES.,RP-DLLME Crude oil AR, Crude oil VR, alkaline and alkaline-earth metals; ICP-OES.,RP-DLLME,Crude oil AR,Crude oil VR,Alkaline and alkaline-earth metals,ICP-OES*

Highlights

RP-DLLME was developed for extraction of alkaline and alkaline-earth metals from crude oil AR and VR. Using 3 g of crude oil AR and VR, the LOD and LOQ were 0.016 and 0.067 µg g^{-1}, respectively.

Resumo/Abstract

The presence of alkali and alkaline-earth metals in crude oil atmospheric (AR) and vacuum residues (VR) can negatively affect refining processes by poisoning catalysts and deactivating acid sites[1]. In this study, a reversed-phase dispersive liquid-liquid microextraction (RP-DLLME) method was developed for further determination of Ca, K, Mg, Na, and Sr in crude oil AR and VR by ICP-OES. Microwave-assisted wet digestion (MAWD) following ASTM D7876:13(2018)[2] was used to obtain reference values by ICP-OES. Calcium, K, Mg, Na, and Sr determination was performed using an inductively coupled plasma optical emission spectrometer with axial view (Optima 4300 DV, PerkinElmer, United States). Key operational parameters were optimized, including the solvent for crude oils AR and VR solubilization (acetic anhydride, acetic acid, vaseline, toluene, and kerosene), use of isopropyl alcohol as dispersant, sample mass (1 to 5 g), extractant concentration (0.5, 1.0, and 2.0 mol L^{-1} HNO_3), and centrifugation time (5 to 20 min). Optimal conditions were achieved using 3 g of crude oils AR and VR dissolved in 5 mL of toluene, with a mixture of 500 µL isopropyl alcohol and 500 µL of 2.0 mol L^{-1} HNO_3, at 75 °C and 20 min centrifugation. No statistically significant difference was observed between RP-DLLME and MAWD results (t-test, 95% confidence level). The proposed RP-DLLME method provided low limits of quantification (0.016 to 0.067 µg g^{-1}) due to high sample mass, diluted extracts, and low blank values. RP-DLLME proved to be a simple, rapid, and effective sample preparation approach for trace-level determination of alkali and alkaline-earth metals in crude oil residues, while also aligning with green chemistry principles through reduced reagent consumption and simple instrumentation.

[1]Stratiev D, et al., 14 (2024) 14090616.

[2]American Society for Testing and Materials: ASTM (D7876:13(2018), 2018.

Agradecimentos/Acknowledgments

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Evaluation of spectral interferences and absorptive behavior of folic acid in HDES-based microextraction systems

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Palavras Chave:*Hydrophobic deep eutectic solvent,Folic acid,UV-Vis spectrophotometry,Molar absorptivity enhancement*

Highlights

The eutectic system acts as a spectroscopic modifier, increasing the analyte's molar absorptivity.

HDES dual role as extractant and sensitivity enhancer improves microextraction performance.

Resumo/Abstract

Hydrophobic deep eutectic solvents (HDES) have emerged as powerful alternatives to traditional organic solvents in microextraction techniques. Beyond their efficiency as extractants, these systems can significantly influence the spectroscopic behavior of analytes, potentially shift absorption maxima and alter molar absorptivity. This study investigates the impact of an HDES based on trioctylmethylammonium chloride and isoamyl alcohol on the spectrophotometric response of folic acid.

The spectral behavior of HDES and its components was characterized via UV-Vis spectrophotometry (200–800 nm, n=10) to identify potential analytical interferences. Additionally, a partition test using 300 µL of DES in 5 mL of ultrapure water was performed to evaluate the organic-to-aqueous phase transfer.

The molar absorptivity coefficients (ε) for folic acid were experimentally determined based on the Beer-Lambert law, derived from the slopes of analytical curves. Standard solutions were prepared in a 0.1 mol.L^{-1}NaOH solution in the concentration range of 1.0 to 20.0 µg.mL^{-1} both to initial characterization in 0.1 mol.L^{-1} NaOH and to the extraction method using a vortex-assisted dispersive liquid-liquid microextraction.

Spectrophotometric analysis revealed an HDES absorption band between 257 and 283 nm - largely due to the partial transfer of isoamyl alcohol to the aqueous phase. Consequently, the wavelength of 370 nm was shown to be a reliable window for analyte quantification as the HDES background signal is minimal in this region. Comparisons between aqueous solutions and HDES extracts indicated an increase in the molar absorptivity of folic acid in the eutectic system.

Such results highlight that the HDES serves a dual role: it is both an extraction phase and a spectroscopic modifier that directly enhances method sensitivity. These insights underscore the necessity of thorough spectroscopic characterization when developing analytical methods centered on eutectic solvents.

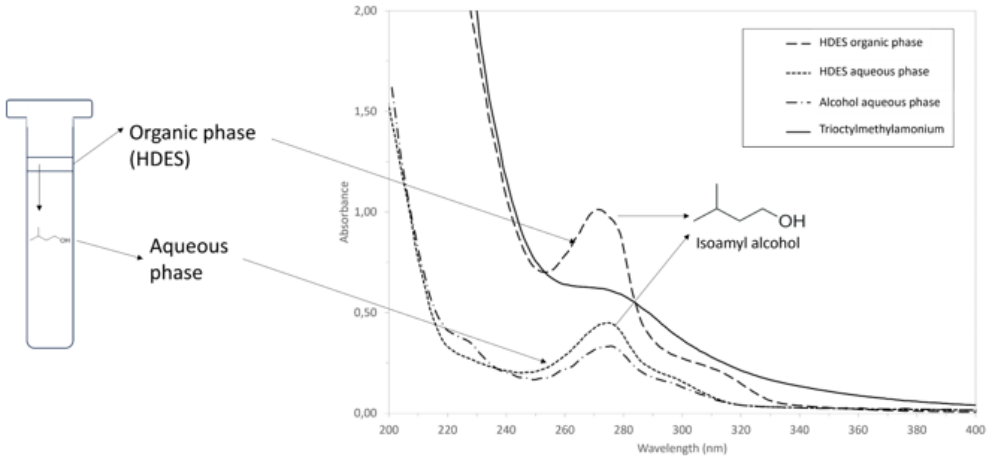


Figure 1 - Spectral comparison between organic and aqueous phases in the HDES system

Explorando vídeos digitais obtidos com smartphone em sistemas de análise por injeção em fluxo para medidas de luminescência

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Palavras Chave:*Luminescência, FIA, smartphone, vídeos digitais,Exploração inédita de vídeos digitais como sistema de detecção em sistema FIA com luminescência, Uso de câmera de smartphone para monitoramento de luminescência.,Luminescência, FIA, smartphone, vídeos digitais*

Highlights

Exploração inédita de vídeos digitais como sistema de detecção em sistema FIA com luminescência, Uso de câmera de smartphone para monitoramento de luminescência.

Resumo/Abstract

A análise por injeção em fluxo (FIA) com detecção por luminescência, destaca-se pela elevada sensibilidade, rapidez e potencial de automação, sendo aplicada na determinação de diferentes espécies químicas. A detecção de luminescência é realizada com equipamentos baseados em fotomultiplicadora ou fotodiodo, o qual é menos dispendioso, mas demanda a montagem da instrumentação, necessitando conhecimentos de eletrônica. Nesse contexto, vídeos digitais obtidos com câmeras de smartphones, surgem como uma alternativa simples, acessível e versátil para detecção em sistemas FIA. Neste trabalho, desenvolveu-se um procedimento FIA com detecção por luminescência, explorando vídeos digitais como ferramenta analítica. A aquisição contínua de imagens, permite a detecção ininterrupta do sinal analítico, característica essencial para reações rápidas, permitindo o monitoramento do curso da reação e a otimização das condições experimentais. A intensidade luminosa foi monitorada analisando os quadros extraídos de vídeos de 6 min, usando software desenvolvido em linguagem Python. O canal azul (B) do sistema RGB foi adotado como sinal analítico, visto que a emissão do luminol ocorre em torno de 426 nm. Como prova de conceito, realizou-se a determinação de peróxido de hidrogênio em água oxigenada de uso farmacêutico, explorando a oxidação do luminol catalisada por ferrocianato de potássio. O método é linear entre 10 e 75 µmol L^{-1} (R^2 > 0,99), apresentado coeficiente de variação de 1,3% (n = 10) 50 µmol L^{-1} de peróxido. Testes de adição e recuperação apesentaram valores entre 83 e 97%, indicando ausência de efeito de matriz. A exatidão foi avaliada comparando com o valor rotulado, apresentaram erros relativos entre 3,7 e 7,4%. Os resultados demonstram que a detecção por vídeos digitais, é uma alternativa viável e de baixo custo como sistema de detecção para FIA, baseado em luminescência, e desta forma contribuindo para a obtenção de métodos analíticos portáteis e de baixo custo.

Agradecimentos/Acknowledgments

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EXPLORING ENANTIOSEPARATION OF ORGANIC UV FILTERS ACROSS CHIRAL STATIONARY PHASES USING LC AND COMPLEMENTARY SFC

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Palavras Chave:*Keywords: Enantioseparation,Chiral stationary phases,Supercritical fluid chromatography,Multimodal liquid chromatography,Organic UV filters,Enantioseparation*

Highlights

LC and SFC screening of five UV filters on 20 CSPs; Baseline enantioseparation for enzacamene, octisalate, homosalate, octinoxate; SFC delivered faster runs and lower solvent use for chiral methods.

Resumo/Abstract

Organic UV filters are widely used in personal care products and are increasingly detected in environmental samples. When these compounds are chiral, treating them as single achiral analytes can mask enantiomer-dependent differences relevant to environmental behavior and risk assessment. In this study, we developed a multimodal screening workflow to identify suitable enantioseparation conditions for five chiral organic UV filters: enzacamene, homosalate, octisalate, octinoxate, and octocrylene. Twenty polysaccharide-based chiral stationary phases, including coated and immobilized amylose- and cellulose-derived columns, were evaluated. In liquid chromatography, the screening included normal-phase conditions with hexane combined with ethanol, 2-propanol, or methyl tert-butyl ether; reversed-phase conditions with water/methanol and water/acetonitrile; and polar-organic conditions using methanol, ethanol, 2-propanol, or acetonitrile. In supercritical fluid chromatography, CO_2 was combined with hexane/ethanol co-solvent mixtures to modulate elution strength and chiral recognition. Separation performance was assessed using a semiquantitative classification of peak separation developed in this study and summarized through separation efficiency metrics. The screening generated 845 chromatograms and showed that enzacamene and homosalate were the most successfully resolved analytes, whereas octocrylene was the most difficult. Normal-phase LC provided the highest number of successful separations, while SFC showed complementary selectivity and performance comparable to LC for several analytes. Overall, amylose-based phases gave the most consistent results, and immobilized chloromethylphenylcarbamate selectors, especially CHIRALPAK IG, showed the broadest applicability. This strategy provides a practical and efficient route for chiral method development and supports enantioselective analysis of organic UV filters in analytical and environmental studies.

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Extração de elementos metálicos em alimentos à base de plantas utilizando solventes eutéticos profundos: um estudo preliminar

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Palavras Chave:*Solventes eutéticos profundos,Extração de elementos metálicos,ICP OES,Alimentos à base de plantas,Química Verde*

Highlights

DES were applied to metal extraction from plant-based foods.

Extraction efficiency showed limited dependence on solvent composition.

Promising results were obtained following Green Chemistry principles.

Resumo/Abstract

A crescente adoção de dietas baseadas em alimentos à base de plantas tem ampliado a necessidade de métodos analíticos confiáveis para a determinação de elementos metálicos, visando à qualidade nutricional e à segurança alimentar. No entanto, métodos convencionais baseiam-se em digestão ácida, com uso de reagentes agressivos e geração de resíduos tóxicos, em desacordo com os princípios da Química Verde. Nesse contexto, solventes eutéticos profundos (DES) surgem como alternativas promissoras.

Este trabalho avaliou o uso de DES no preparo de amostras de alimentos à base de plantas para a determinação de elementos metálicos. Três DES à base de cloreto de colina e ácidos carboxílicos (málico, cítrico e tartárico) foram aplicados na extração de Ca, Cu, Fe, K, Mg, Mn e Zn de quatro alimentos vegetais (1-almôndega, 2-mistura para hambúrguer, 3-nugget e 4-proteína de soja texturizada). As amostras foram secas, moídas, submetidas à extração em banho ultrassônico (60 °C, 30 min) e analisadas por ICP OES.

Os resultados, ainda que preliminares, indicaram pequenas variações na eficiência de extração em função da composição do DES, com diferenças pouco expressivas entre os solventes. De modo geral, o DES à base de cloreto de colina e ácido cítrico apresentou desempenho ligeiramente superior para a maioria das matrizes e elementos.

As concentrações variaram conforme o alimento analisado. Para Ca, os teores situaram-se entre ~60 e 160 mg/100 g (base úmida) nas amostras 1, 2 e 3, alcançando cerca de 2000 mg/kg (base seca) na proteína de soja. O K apresentou as maiores concentrações (~200–800 mg/100 g e >14 000 mg/kg), enquanto Mg foi observado em níveis intermediários (25–123 mg/100 g e ~2000 mg/kg). Cu, Mn e Zn ocorreram em concentrações inferiores (0,1–8 mg/100 g e 10–70 mg/kg).

Os resultados indicam que os DES apresentam desempenho consistente na extração de elementos metálicos em alimentos à base de plantas, constituindo uma alternativa mais sustentável para análises de alimentos.

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Feasibility of using methanesulfonic acid for metal leaching from silver oxide button cell waste

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Palavras Chave:*waste valorization,valuable metals,green chemistry,green leaching,organic acid.*

Highlights

Spent button batteries are a source for valuable metal recovery. Methanesulfonic acid is a viable and effective alternative for green metal leaching from spent button batteries.

Resumo/Abstract

Silver oxide (Ag_2O) button cells are used in portable electronic devices, such as digital wristwatches. Recovering metals such as silver, zinc, manganese, and nickel from the waste of these batteries is a way to minimize current economic and environmental problems. Therefore, this work aims to investigate the feasibility of leaching these metals from button cell waste using methanesulfonic acid (MSA) as a leaching agent, as MSA is considered a green acid and a promising tool for advancing more sustainable chemistry[1]. To determine the optimal experimental leaching conditions, a Central Composite Rotatable Design (CCRD) with 3 variables was employed, yielding 17 runs. The investigated variables were temperature (25 to 75 °C), solid-liquid ratio (0.025 to 0.100 g g^{-1}), and MSA concentration (0.10 to 2.0 mol kg^{-1}). Leaching time and stirring speed were kept constant at 2 h and 600 rpm, respectively. The metals present in the leachate obtained in each experimental run were quantified by Total Reflection X-Ray Fluorescence Spectrometry. The analysis of the CCRD results showed that higher MSA concentration and temperature values yield greater leaching efficiency for all metals, due to increased proton availability and stronger molecular interactions. Conversely, a higher solid-liquid ratio negatively affects leaching efficiency by reducing the effective interaction area due to the greater amount of solid relative to the liquid. Thus, a temperature of 65 °C, MSA concentration of 2.0 mol kg^{-1}, and solid-liquid ratio of 0.04 g g^{-1} were the best conditions for leaching, yielding (86±2), (78±1), (93±2), (95±2) % for Ag, Mn, Zn, and Ni, respectively. These results were consistent with the theoretical indications of the CCRD. Thus, the potential of using dilute MSA solution and milder temperatures for more sustainable metal leaching from Ag_2O button cell waste was demonstrated, highlighting this waste as a strategic secondary source of silver.[1]Green Chem.,2024,26,8583.

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Firearm and Ammunition Differentiation from Gunshot Residue Using SEM/EDX and Machine Learning

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Palavras Chave:*Gunshot residue,SEM/EDX,forensic analytical chemistry,machine learning,ballistic discrimination*

Highlights

SEM/EDX elemental fingerprints enable objective firearm and ammunition discrimination. Machine learning achieved >80% accuracy in multiclass GSR classification.

Resumo/Abstract

Gunshot residue (GSR) is a complex particulate system originating from primer compounds, projectile materials, firearm components, and environmental substrates transferred during a ballistic event. Although conventional studies prioritize compositional characterization and standardization, this work emphasizes the analytical discrimination of firearms and ammunition types through quantitative elemental profiling combined with machine learning.

Experimental data were generated in partnership with the Federal Police. Three calibers (9 mm, .357, and .38) were fired in triplicate at a white cotton T-shirt positioned two meters from the muzzle using jacketed, bare lead alloy, and semi-jacketed projectiles. GSR particles were characterized by scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM/EDX). For each shot, eight microscopic fields were randomly analyzed with seven point measurements per field, producing 56 elemental observations per firearm.

Descriptive chemometric assessment focused on oxygen (O) and carbon (C), associated with combustion-derived residues, and lead (Pb), indicative of projectile composition. Incomplete elemental profiles were excluded to improve data integrity and model robustness. Supervised classification models were constructed using PyCaret, enabling systematic benchmarking of 15 algorithms. Ensemble and non-linear classifiers exhibited superior performance relative to linear models, achieving classification accuracies exceeding 80% and demonstrating strong discrimination capability.

The integration of SEM/EDX elemental fingerprints with machine learning provides a robust analytical framework for objective firearm and ammunition differentiation. This approach enhances evidential interpretation of ballistic microtraces, reduces subjectivity in forensic assessments, and supports the advancement of quantitative forensic analytical chemistry.

Agradecimentos/Acknowledgments

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Green synthesis of silver nanoparticles using Syzygium cumini leaf extract and AgNO3 from recovered silver: temperature effect

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Palavras Chave:*Silver nanoparticles,Recovered silver,Green synthesis,Syzygium cumini,UV-Vis*

Highlights

AgNPs synthesized via Syzygium cumini leaf extract and recovered-silver $AgNO_3$.

Alkaline pH speeds nucleation and stabilizes colloids.

80°C boosts SPR and shifts λ_{max} (~405–416 nm) in 60 min (UV–Vis).

Resumo/Abstract

Green synthesis of silver nanoparticles (AgNPs) is a sustainable alternative to conventional routes, using plant extracts as reducing and stabilizing agents. We investigated AgNP biosynthesis using an aqueous Syzygium cumini (Myrtaceae) leaf extract, focusing on the temperature effect on formation kinetics, and employing $AgNO_3$ prepared from silver recovered from laboratory residues.

Leaves were washed, dried (40 °C, 48 h), ground, and extracted in distilled water (10 g/50 mL, 90 °C, 30 min). The extract was filtered, stored at 4 °C, and used within 24 h. A recovered $AgNO_3$ salt (95% w/w) was used to prepare $AgNO_3$ (1 mmol L^{-1}; initial pH 5.3). For synthesis, 1 mL of extract was added to 50 mL $AgNO_3$, the medium was adjusted to pH 9.0, and two conditions were tested: 25 °C and heating (75–85 °C). Formation was monitored by UV–Vis every 15 min up to 60 min.

A color change to dark brown indicated Ag^+ reduction. UV–Vis spectra showed the surface plasmon resonance (SPR) band (400–420 nm; Figure 1). At 25 °C, λ_{max} ~416 nm with low intensity was observed, whereas under heating the band shifted to ~405 nm with markedly higher absorbance (~2.7 vs ~1.0 a.u.), indicating faster formation and improved dispersion, consistent with reports that alkaline pH (~9) promotes nucleation and colloidal stability [1,2]. Measurements beyond 75 min exceeded the spectrophotometer absorbance range; therefore, results are reported up to 60 min to keep comparisons within the instrument's linear window.

Overall, S. cumini leaf extract efficiently mediates green AgNP synthesis from recovered silver, and temperature is a key kinetic driver: heating yields more dispersed, stable nanoparticles in shorter times, supporting future applications in analytical chemistry (sensing and conductive materials).

Refs.: [1] Sekhar et al., J. Appl. Pharm. Sci. v. 8, n. 1, p. 073-079, 2018; [2] Hombalimath et al., Asian J. Pharm. v. 19, n. 3, 2025.

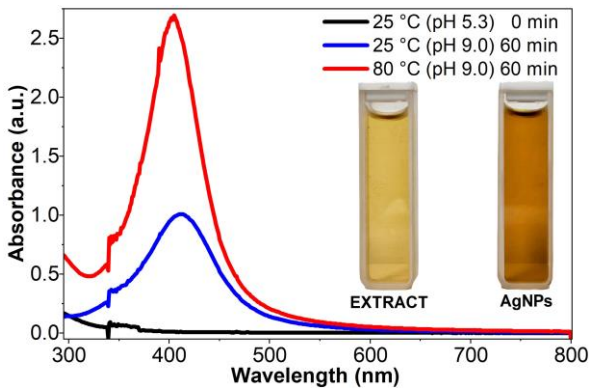


Figure 1. UV-Vis absorption spectra of AgNPs synthesized using Syzygium cumini leaf extract.

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Immersive simulation of microtraces as a tool for pre-analytical standardization in Forensic Evaluation.

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Palavras Chave:*Augmented Reality; Crime Scene Simulation; Trace Evidence; Forensic Training; Pre-analytical Uncertainty*

Highlights

AR-based crime-scene simulation enhances trace evidence evaluation;
It reduces uncertainty in forensic pre-analytical procedures.

Resumo/Abstract

Collecting microtraces at crime scenes is essential for forensic accuracy due to small samples, contamination risks, and strict protocols. The pre-analytical phase introduces uncertainty affecting analysis, traceability, and chain-of-custody. Traditional simulations face issues with reproducibility, standardization, cost, and waste. Using Augmented Reality (AR) offers controlled simulations with virtual overlays. This study assesses AR's feasibility for crime-scene simulation, focusing on trace-evidence handling. A systematic literature review was conducted to map current practices in forensic training, crime-scene simulation, and immersive technologies. Searches were performed in Web of Science, Google Scholar, SciELO, and ScienceDirect for publications between 2015 and 2025 using the keywords “Forensic Training,” “Crime Scene Simulation,” “Augmented Reality,” and “Trace Evidence.” The search retrieved 944 records. Studies were included if they were peer-reviewed articles published in English or Portuguese dealing with forensic training, crime-scene simulation, or immersive technologies related to trace-evidence handling or scene processing. They were excluded if they: (i) focused only on legal or argumentative topics without field forensic relevance; (ii) covered macroscopic investigation aspects like body positioning or ballistic trajectories without trace-evidence or immersive tech focus; or (iii) lacked full text or scientific rigor, such as editorials and abstracts without complete methods. After removing duplicates and screening, 38 studies were analyzed. Based on these findings, an AR simulation environment was implemented using the Meta Quest 2 platform. The analyses indicate stable visualization of virtual evidence in physical environments and satisfactory usability. Overall, AR represents a promising complementary approach for crime-scene simulation and improved reliability in trace-evidence handling.

Study selection process according to the PRISMA protocol.

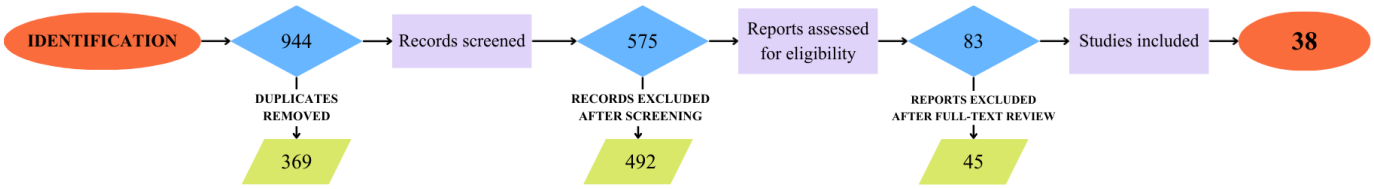


Figure 1. Flowchart of the study selection process based on PRISMA

Agradecimentos/Acknowledgments

1. Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, PIBIC e INCT-SP: 406958/2022-0.
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3. Programa Unificado de Bolsas da USP

Improving the Accuracy of Phenolic Quantification in Fruit Extracts Using a Microvolume Folin–Ciocalteu Assay

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Palavras Chave:*Total phenolic content, matrix effects, microplate colorimetric assay, method miniaturization, antioxidant activity*

Highlights

The miniaturized method provides faster results with less reagent use.

Matrix effects were mitigated by pre- and post-alkalization readings, improving the method's accuracy and reproducibility.

Resumo/Abstract

Phenolic compounds are widely distributed in fruits and are closely associated with antioxidant activity. The Folin-Ciocalteu (F-C) method is commonly used for quantifying phenolics; however, variations in reaction conditions and matrix effects can lead to overestimation of results. Furthermore, the conventional application of this method requires a relatively high volume of reagents, generating substantial waste. In this sense, this study aimed to develop a miniaturized F-C method using a microplate reader. For this, six fruit extracts such as mango, guava, pomegranate, and araticum were used. The effects of wavelength, reaction time, reagent ratios, and sample volume were evaluated. The results showed that the overestimation of phenolics arises from matrix effects caused by reducing compounds reacting with the molybdate and tungstate complexes of the F-C reagent. By implementing two absorbance measurements, one before alkalization of the medium and another after the reaction progressed, analytical accuracy was significantly improved, even in matrices with a high content of interferents. The optimized conditions were: volume adjustment (190 µL of water, 15 µL of sample, 15 µL of F-C reagent, and 30 µL of Na_2CO_3); reaction time of 120 min; and absorbance measurement at 725 nm. The limits of detection and quantification were 0.002 and 0.005 mg/mL, respectively. Standard-addition experiments at three levels yielded recoveries within the 80% to 120% range, and the relative standard deviation for all measurements was below 8%. Additionally, antioxidant activity was determined using the DPPH radical scavenging assay, a useful indicator of matrix effects that enables identification of samples susceptible to phenolic overestimation. In summary, the proposed method proved simple, efficient, reproducible, and suitable for microplate analysis, effectively minimizing overestimation of results and waste generation, while enabling simultaneous quantification of multiple samples.

Agradecimentos/Acknowledgments

The authors thank the Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG, APQ-01460-25, APQ-04528-23) for funding.

Influence of different selenium species on the early development of Lettuce Seedlings (Lactuca sativa L.)

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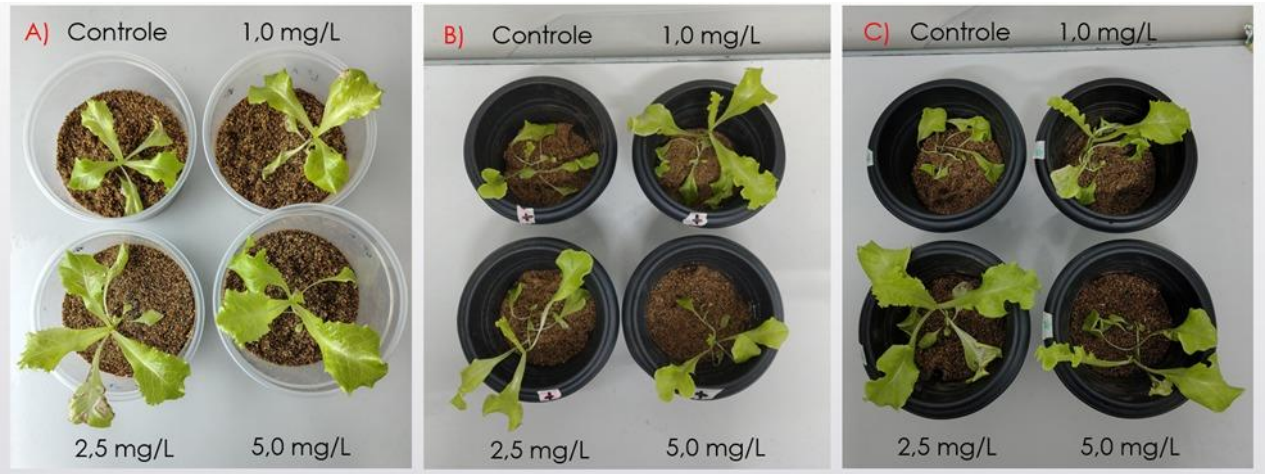
Palavras Chave:*Alface, Cultivo, Vermiculita, Nanotecnologia, Agricultura.*

Highlights

Lettuce seeds exposed to SeNPs showed reduced water consumption and improved early growth. Increased fresh mass, shoot, root, and leaf development were observed at specific concentrations.

Resumo/Abstract

Diante da crescente demanda por alimentos nutricionais para suprir as necessidades fisiológicas humanas, a busca por novas tecnologias para melhoria no setor agrícola, torna-se essencial. Uma abordagem promissora envolve a inserção de nutrientes desde as fases germinativas das plantas como um estímulo à produtividade e aumento do teor nutricional dos alimentos, a exemplo da alface, de amplo consumo na dieta humana (FAO*et al*., 2023). O presente estudo avaliou o desenvolvimento de mudas de alface anteriormente expostas a diferentes espécies de selênio, tais como selenito (Se(IV)), selenato (Se(VI)) e nanopartículas de selênio estabilizadas com quitosana (SeNPs_QUI) (Se⁰) (Neta*et al*., 2026). Para tanto, mudas de alface expostas a concentrações de selênio de 1; 2,5 e 5 mg/L (N = 6), foram adicionadas em potes de polipropileno contendo 80 g de vermiculita, umedecida com 250 mL de água deionizada e submetidas a ciclos de iluminação de 12h (presença/ausência de luz). Ao longo do período de cultivo, as alfaces foram regadas com água deionizada e solução nutritiva de Hoagland a 5% em distintas quantidades, a depender da necessidade das amostras. Os resultados indicaram que a exposição das sementes às SeNPs e Se(IV) afetou o consumo hídrico da hortaliça, demonstrando menor consumo de água nas amostras expostas a maiores concentrações. As amostras de 5mg/L expostas a SeNPs obtiveram um melhor resultado quanto ao desenvolvimento de tamanho da hortaliça, entretanto nas amostras expostas a Se(IV) e Se(VI) para a mesma concentração houve uma diminuição do desenvolvimento da hortaliça, indicando um possível efeito fitotóxico em concentrações superiores a 2,5 mg/L. Entretanto, se faz necessário investigar a composição mineral para uma avaliação nutricional das plantas.



Amostras expostas a diferentes concentrações de selênio: A) SeNPs_QUI; B) Se(IV); C) Se(VI).

Agradecimentos/Acknowledgments

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In Silico Strategies for Predicting NPS Metabolites: A systematic review

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Palavras Chave:*New psychoactive substances, In silico metabolism, Analytical chemistry, Metabolite prediction*

Highlights

Systematic review on in silico strategies for NPS metabolite prediction. Computational access to toxicological and structural properties can drive analytical analysis, reducing time and cost.

Resumo/Abstract

New Psychoactive Substances (NPS) represent an analytical challenge for forensic and toxicological laboratories due to their rapid structural diversification and the absence of reference standards for both parent compounds and metabolites. After consumption, NPS undergo extensive biotransformation, mainly mediated by cytochrome P450 enzymes, generating metabolites that serve as key analytical targets for detection, identification, and interpretation of exposure. Conventional in vitro and in vivo metabolism studies are time-consuming, costly, and often incompatible with the pace of NPS emergence in illicit markets. In this context, in silico tools have gained prominence as complementary analytical strategies for predicting metabolic pathways, prioritizing target metabolites, and supporting the development of analytical methods based on chromatographic and mass spectrometric techniques. This study presents a systematic literature review on the application of in silico approaches to predict metabolites and toxicological profiles of amphetamines, synthetic cannabinoids, and phenethylamines compounds. Searches were conducted in Web of Science, Dimensions, PubMed, and Scopus using the keywords “metabolites,” “in silico,” and specific NPS names combined with the Boolean operator “AND.” The results indicate a substantial growth in publications related to amphetamines and synthetic cannabinoids, reflecting their analytical relevance and the increasing incorporation of computational tools to guide metabolite identification workflows. Although phenethylamines derivatives compounds present lower publication numbers, a rising trend suggests expanding analytical interest. Overall, in silico metabolism prediction emerges as a cost-effective and time-efficient analytical resource, capable of supporting method development, improving target selection for instrumental analysis, and enhancing the robustness of analytical strategies applied to emerging drugs.

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1. Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, PIBIC e INCT-SP: 406958/2022-0.

2. Coordenação para o Aperfeiçoamento de Pessoal de Nível Superior: (CAPES, Financial Code 001).

Intelligent Spectral Platforms for Forensic NPS Identification: A PRISMA-Based Review

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Palavras Chave:*New Psychoative Substances,Machine Learning,Spectroscopic techniques*

Highlights

PRISMA review highlights machine learning in IR and MS for emerging drugs.
Predictive models improve classification beyond spectral libraries.
Digital systems can support forensic decisions.

Resumo/Abstract

The rapid emergence of new psychoactive substances (NPS) presents significant challenges for forensic analytical chemistry due to continuous structural modifications, a scarcity of certified reference materials, and incomplete spectral libraries. These issues hinder both presumptive screening and confirmatory identification, impacting the accuracy and reliability of analyses and evidence. This systematic review, conducted according to PRISMA guidelines, examines studies published between 2009 and 2025 in the ScienceDirect, Google Scholar, and SciELO databases. It focuses on the main categories of NPS, such as amphetamines, synthetic cathinones, fentanyl analogs, phenethylamines, and synthetic cannabinoids, highlighting especially infrared (IR) spectroscopy and mass spectrometry (MS), combined with machine learning (ML) and chemometrics, for compound differentiation. Forty-three articles were eligible for evaluation. The results demonstrate that data-driven spectral interpretation via ML can aid classification compared to traditional library matching, especially in complex mixtures and between structurally related analogs. Predictive models can facilitate rapid screening and offer adaptive updates as new substances emerge. Based on these advancements, a digital prototype is proposed that combines public spectral databases with machine learning-based decision support. This system is being tested through simulated workflows, using PDCA (Plan-Do- Check-Act) and SWOT (Strengths, Weaknesses, Opportunities, and Threats) analyses to assess robustness, scalability, and operational feasibility. Overall, the review emphasizes the growing importance of intelligent platforms to enhance analytical performance, traceability, and reliability in forensic drug analysis.

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1. Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq INCT-SP: 406958/2022-0.
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3. Coordenação para o Aperfeiçoamento de Pessoal de Nível Superior: (CAPES, Financial Code 001).

Ionomic study of ora-pro-nobis enriched with selenium nanoparticles in hydroponic cultivation.

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Palavras Chave:*Biofortification,Selenium nanoparticles,Ora-pro-nóbis (Pereskia aculeata),ICP-MS,Hydroponic cultivation*

Highlights

Ionomic evaluation of selenium enrichment in ora-pro-nobis under hydroponic cultivation via ICP-MS.

Selenium nanoparticle biofortification of*Pereskia aculeata*leaves using hydroponic cultivation.

Resumo/Abstract

Ora-pro-nóbis (*Pereskia aculeata Miller*) is an unconventional food plant (UFP) used in human nutrition through the consumption of its leaves, which contain significant levels of proteins, fibers, vitamins, and minerals. Due to its easy cultivation, low production cost, and high adaptability to different environmental conditions, this species stands out as a promising plant for selenium agronomic biofortification. In this context, selenium (Se) was chosen due to this element recognized role in antioxidant, immunological, and endocrine functions, particularly in regions where dietary intake is limited. The goal of this study was the evaluation of the biofortification of ora-pro-nóbis with selenium nanoparticles (SeNPs) stabilized with chitosan through hydroponic cultivation, as well as to investigate possible changes in the plant ionomic profile. Cultivation was carried out in Hoagland nutrient solution, with and without substrate, including control groups and treatments with different SeNP concentrations, in addition to a comparative treatment with Se(IV) as sodium selenite. During the experimental period, plant development was monitored through observations of morphological aspects related to growth and adaptation to the different cultivation systems. At the end of the experiment, leaves were collected, washed, freeze-dried, ground to a fine powder, and subjected to microwave-assisted acid digestion. The determination of Se, Al, Cu, Mn, Zn was performed by inductively coupled plasma mass spectrometry (ICP-MS). Based on a method with an estimated limit of quantification (LOQ) of approximately 0.20 mg/kg and a selenium recovery between 70% and 130% for the certified reference material NIST 1573a, the results showed the translocation of the Se to the leaf and its enrichment, where we can observe a translocation of Se-NPs approximately three times higher than that of Se(IV) under the best cultivation condition identified.



Ora-pro-nóbis seedlings in hydroponic cultivation during the experiments period.

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IR spectroscopy applied to hormone-based medications and psychiatric drugs classification through SIMCA

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Palavras Chave:*Forensic science,chemometrics,infrared spectroscopy,hormone-based drugs,psychiatric drugs*

Highlights

Hormone and psychiatric drugs characterization using DFT calculations. SIMCA method applied to the development of classification models.

Resumo/Abstract

The use of hormone-based pharmaceuticals and psychotropic drugs has increased significantly in recent years. Consequently, the production and commercialization of these compounds have intensified, both within the pharmaceutical industry and in society. Moreover, several of these substances may be consumed as drugs of abuse and may also act as environmental micropollutants, causing ecological imbalance. Therefore, the characterization and identification of hormonal and psychotropic compounds are of considerable relevance[1]. Experimental techniques are often unable to address the large number of samples requiring analysis, due to limitations related to instrumentation, infrastructure, or the availability of suitable reference standards. In this context, in silico methods represent viable alternatives to complement experimental approaches. Computational chemistry methods enable the generation of reliable data capable of accurately describing chemical systems[2]. In this study, Density Functional Theory (DFT) was applied to perform geometry optimizations on a dataset comprising 30 hormonal pharmaceuticals and 30 psychotropic drugs. Vibrational frequency calculations were also carried out, allowing the generation of theoretical infrared spectra. These spectra, with wavenumbers ranging from 400 to 4000 cm^{-1}, were used as molecular descriptors for this system[3]. The chemometric method Soft Independent Modeling of Class Analogy (SIMCA) was then employed for molecular classification. The model successfully classified the compounds as hormones or psychotropic drugs and identified subclasses such as androgens, glucocorticoids, benzodiazepines, and tricyclic antidepressants. These results indicate that computational methods are valuable auxiliary tools in environmental and forensic applications.

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Melofen-derived urease inhibitors: in vitro, in silico and biophysical studies

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Palavras Chave:*Urease. Melofen,Inhibitors,Improved fertilizers,antimicrobials,in silico and in vitro studies*

Highlights

Melofen-type derivatives exhibited promising antiureolytic activity*in vitro*and in soil assays but demonstrated low efficacy against ureolytic fungi and bacteria

Resumo/Abstract

Urease is a fundamental enzyme in the nitrogen cycle, widely studied due to the impacts of rapid urea hydrolysis, both in agricultural soils and in the health field.2 Thus, in this work, the antiureolytic activity of melofen derivatives (Fig. 1A) was investigated in vitro and in silico systems. The results showed that NBPT was the most potent inhibitor in solution (Fig. 1B), but its effectiveness decreased in the presence of humic substances (HS), while melofen derivatives, especially M4, maintained stability in soils (Fig. 1C). Soil tests (M1 and M3) outperformed NBPT (Fig. 1D). Kinetic analyses confirmed competitive inhibition (Fig. 1E-F), with KI of 0.36 ± 0.01 µM (without HS) and 0.23 ± 0.01 µM (with HS). UV-Vis spectroscopy revealed the formation of the M1-Ni^{2+} complex (Fig. 1G), with kb = 2.37 x 10^3 L mol^{-1}, indicating moderate interaction. Furthermore, Ellman assays showed a reaction of M1 with free thiol groups in models with AMP and cysteine (Fig. 1H-I). 3D fluorescence demonstrated that M1 leads to conformational changes in the urease structure (Fig. 1J-K). Molecular docking corroborated these results, indicating the interaction between M1 and Ni^{2+} and thiol groups at the site near the urease site (Fig. 1L). In addition, derivatives M1 and M2 were bacteriostatic against S. aureus and E. coli, while M1 was fungistatic against C. neoformans and C. albicans. M3 and M4 did not demonstrate bactericidal activity, being fungistatic mainly against C. neoformans. No compound showed bactericidal or fungicidal action. Thus, melofen derivatives showed relevant activities that could be explored mainly for agricultural purposes and in the design of more active substances.

Reference: 1Viana et al. Bioorganic Chemistry. 146. 107247. 2024. 2Morais Costa et al. Bioorganic Chemistry. 152. 2024. 107735. 2024

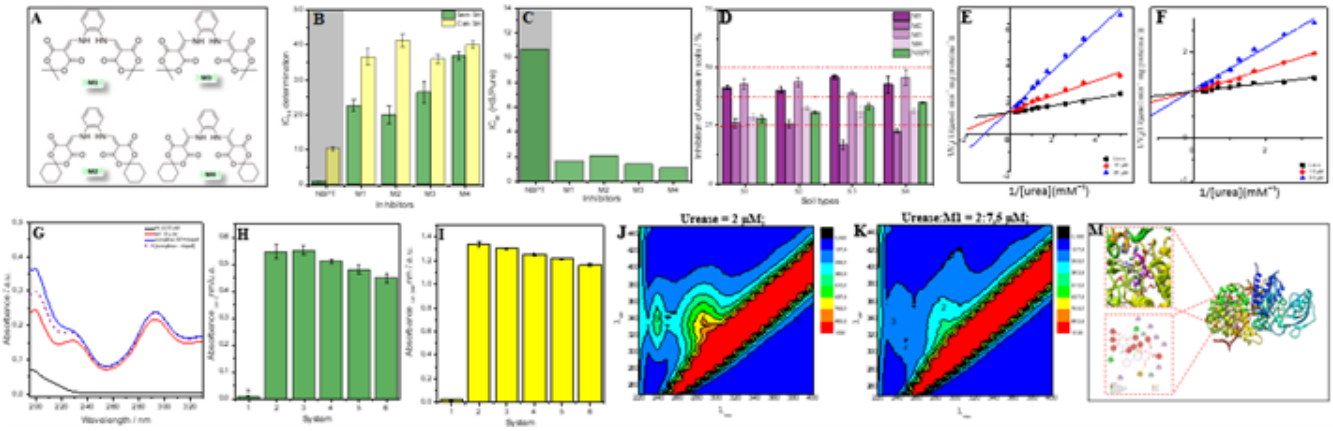


Fig. 1. Experimental results of urease inhibition tests by melofen derivatives

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Metabolomic profiling of psychedelic mushrooms by LC-HRMS

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Palavras Chave:*Psilocybe cubensis,Amanita muscaria,Metabolomics,Mass spectrometry,Sample preparation*

Highlights

Untargeted metabolomic analysis of Amanita muscaria and Psilocybe cubensis using comparative profiling to reveal metabolites with potential interactive effects by high-resolution mass spectrometry.

Resumo/Abstract

Psychedelic compounds such as psilocybin have attracted increasing interest due to their therapeutic potential in neuropsychiatric disorders, including major depressive disorder, substance use disorders, post-traumatic stress disorder, and possibly dementias. Psilocybin is found in mushrooms of the Psilocybe genus, such as*Psilocybe cubensis*, and previous studies have reported the presence of additional alkaloids that may contribute to combined or complementary biological effects. Other species, including, exhibit psychoactive properties due to compounds associated with toxicity. In this study, a biphasic extraction protocol (MTBE:MeOH:water 10:3:2) was applied to perform an untargeted metabolomic comparison between a wild sample of*Amanita muscaria*and samples of*Psilocybe cubensis*cultivated on four different substrates. Metabolic profiling was carried out using liquid chromatography coupled to an Orbitrap high-resolution mass spectrometer (Exploris 120, Thermo Scientific) with both an Acquity UPLC BEH Amide and Acquity UPLC BEH C18 columns (Waters, 2.1 x 100 mm; 1.7 µm) aiming to identify additional bioactive metabolites and to evaluate the influence of cultivation substrate on mushroom metabolism.

Metal recovery from spent nickel-metal hydride batteries using methanesulfonic acid

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Palavras Chave:*Experimental design,Organic acid,Recycling,Rare earth elements,Electronic waste*

Highlights

The recycling of NiMH batteries is promising for the recovery of strategic metals; Methanesulfonic acid showed promising results, with high leaching efficiencies under mild conditions.

Resumo/Abstract

The demand for nickel-metal hydride (NiMH) batteries has grown due to their wide application in portable electronic devices and hybrid and electric vehicles. These batteries contain strategic metals, which are essential to various production chains. When obsolete, improper disposal can cause significant environmental impacts, in addition to representing the loss of valuable materials in high demand and limited supply. This study evaluated the dissolution of metals present in the anodic material of NiMH batteries using methanesulfonic acid (MSA) as a leaching agent. A central composite rotational design (CCRD) was applied to investigate the effects of temperature (25–75 °C), solid–liquid ratio (0.03–0.08 g mL^{-1}), and MSA concentration (0.16–1.84 mol L^{-1}) on the leaching of metals, and consequently to optimize the leaching process. Time and stirring speed were kept constant at 240 min and 600 rpm. The reproducibility of the process was evaluated through a triplicate of the CCRD central point, under the conditions of 50 °C, a solid-to-liquid ratio of 0.05 g mL^{-1}, and an MSA concentration of 1.0 mol kg^{-1}. Leachates were analyzed by total reflection X-ray fluorescence spectrometry and microwave-induced plasma atomic emission spectrometry, employing internal standard and standard addition calibration, respectively, to quantify metals. The leaching efficiency obtained for Ni, Mn, Co, La, Ce, Zn, Y, and Cu were 67, 86, 82, 86, 86, 84, and 82 %, respectively, with a coefficient of variation ranging from 2 to 4 %, indicating good reproducibility. Tests at the CCRD axial points demonstrated that MSA concentration and the solid-to-liquid ratio influence leaching efficiency. Meanwhile, temperature shows a lower impact when the leaching efficiency exceeds 70 %. The results obtained indicate that the proposed process is efficient for recovering metals from discarded NiMH batteries and serves as an alternative to the use of conventional strong acids.

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Metals determination in dental ceramic materials: analytical challenges for method development

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Palavras Chave:*Ceramic materials, metals determination, biocompatibility, microwave-assisted digestion, ICP-OES,Ceramic materials,metals determination,biocompatibility,microwave-assisted digestion, ICP-OES,microwave-assisted digestion,ICP-OES*

Highlights

Sample preparation for hard-to-digest matrices
Microwave-assisted digestion using acid mixtures
Metals determination in dental ceramic materials
Ammonium fluoride to digest refractory matrices

Resumo/Abstract

Ceramic materials are applied in odontology due to their mechanical strength, chemical stability, and biocompatibility. Yttrium oxide is commonly incorporated into these materials to stabilize the crystalline structure, to improve mechanical resistance, and to enhance optical properties. However, inappropriate yttrium concentration or the presence of other metals may compromise material performance and biological safety, making accurate elemental determination essential. The metals quantification in ceramics remains an analytical challenge due to the high chemical stability and resistance of these materials. In this work, six ceramic samples were subjected to microwave-assisted wet digestion (MAWD, Ethos Easy, Milestone, Italy) operating with 44 PTFE vessels, with maximal temperature of 200 °C and 35 bar of pressure. The digestion program was 25 min of ramp to reach 200 °C at 1800 W, maintaining 15 min at 200 °C (1800 W) and 20 min for cooling (0 W down to 50 °C). Two ceramic samples were randomly chosen for sample preparation optimization. Three digestion mixtures were evaluated using concentrated acid solutions for sample mass ranging from 25 to 150 mg:*i*) 3.5 mL HCl + 1.5 mL HF + 1.0 mL HNO_3,*ii*) 3.5 mL HF + 1.5 mL HCl + 1.0 mL HNO_3, and*iii*) 6.0 mL HCl + 2.0 mL HCl + 2.0 mL NH_4F (100 g L^{-1}) with a second digestion step using 20 mL of 4% (m m^{-1}) H_3BO_3. The determination of Ag, Al, Ba, Ce, Cr, Cu, Fe, La, Mg, Mn, Mo, Ni, Pb, Zn, Y, and Zr was carried out using an inductively coupled plasma optical emission spectrometer (ICP-OES, Spectro Ciros CCD, Spectro Analytical Instruments, Germany) equipped with a cross-flow nebulizer coupled to a double pass-Scott type spray chamber. A complete sample digestion (100 mg) was obtained using the acid mixture containing HCl, HNO, NH_4F, and H_3BO_3 for all ceramic samples. The higher content was observed for Y, Zr, and Ce, with content ranging from 3 to 6%, 44 to 50%, and 3.9 to 4.2% (m m^{-1}), respectively, for all samples.

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CNPq, CAPES, and UFSM

Methodological Aspects of ED-XRF Combined with Chemometric Approaches for Assessing Phytoremediation of E-waste Substrates Using Phalaris canariensis

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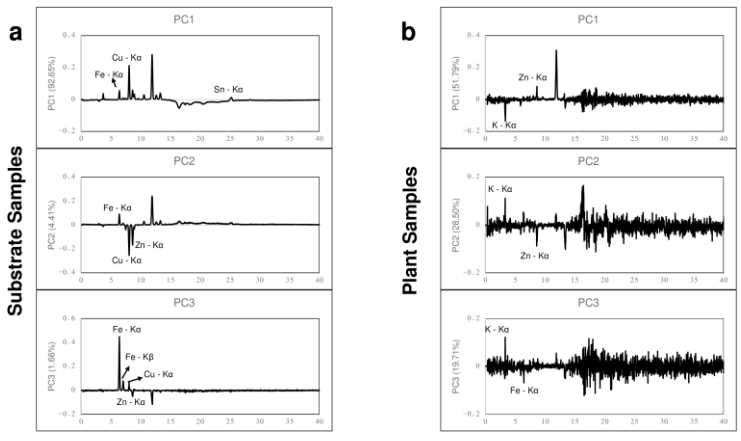
Palavras Chave:*ED-XRF,Toxic metals,Chemometrics,PCBs,Phytoremediation*

Highlights

Assessing the potential of low-cost benchtop ED-XRF combined with chemometrics for phytoremediation studies of metals from e-waste contaminated substrates.

Resumo/Abstract

Introduction: Printed circuit boards (PCBs) are one of the main components of electronic waste, containing toxic metals such Copper (Cu), tin (Sn), zinc (Zn), and lead (Pb) [1]. Phytoremediation is a sustainable remediation technology that uses plants to remove, stabilize, or accumulate metals from contaminated substrates, and in this study, it is coupled with energy-dispersive x-ray fluorescence (ED-XRF), a green chemistry-based analytical technique [2]. This work focuses on the capabilities and challenges of ED-XRF as an analytical tool for investigating the potential of Phalaris*canariensis*for phytoremediation of substrates contaminated with PCB-derived metals, using chemometrics (data science).**Methodology:**For this study, two cultivation conditions were established: a reference system containing only sawdust and Phalaris*canariensis*seeds, and a test system with the addition of ground PCB samples (<53 µm) from discarded smartphones. Seeds were grown under identical conditions, and plant samples were collected at the same growth stage. After drying at 50 °C for 48 h, ED-XRF spectra were acquired using a benchtop spectrometer (Rigaku NEX QC$^+$, Ag tube, SDD) under three excitation conditions (50 kV/10 µA; 30 kV/10 µA; 6.5 kV/50 µA) [3], with data processed in MATLAB®.**Results:**Principal Component Analysis (PCA) applied to ED-XRF spectra revealed distinct methodological performance across sample matrices and preparation methods. For substrate samples, a matrix well suited to powder-base XRF analysis, the first three principal components explained 98.71% of the total variance (PC1: 92.65%, PC2: 4.41%, PC3: 1.66%), indicating strong data structuring and high discriminatory capability, PC1 positive charges were dominated by copper emission line (Cu – Kα), while PC2 and PC3 presented Zn – Kα and Fe – Kα / Fe – Kβ emission lines. In contrast, PCA applied to plant samples analyzed without ideal sample preparation (non-macerated biomass) resulted in a more distributed variance, with PC1, PC2, and PC3 explaining 51.79%, 28.50%, and 19.71% of the variance, respectively, highlighting the influence of sample matrix and preparation on ED-XRF signal quality and chemometric performance in phytoremediation assessments.**Conclusion:**This study demonstrates that ED-XRF, combined with chemometric analysis, is a viable method for assessing phytoremediation, with analytical performance strongly dependent on sample preparation. Powdered matrices, particularly substrates, provided higher data structuring and more reliable chemometric interpretation than non-powdered plant samples, highlighting the importance of preparation protocols in ED-XRF-based environmental studies.



PCA loadings from ED-XRF spectra of (a) substrate and (b) plant samples

Agradecimentos/Acknowledgments

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Microwave Synthesis of Co-MOFs for Ciprofloxacin and Fluoxetine Adsorption.

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Palavras Chave:*Cobalt,MOF,Microwave,Synthesis,Contaminants*

Highlights

Microwave-assisted synthesis of Cobalt-MOFs;

Fast adsorption dynamics within short contact times;

Application of Co-MOFs for ciprofloxacin and fluoxetine adsorption.

Resumo/Abstract

Emerging contaminants (ECs), particularly pharmaceuticals, are persistent aquatic pollutants that are poorly removed by conventional wastewater treatment processes, raising environmental and public health concerns. In this context, this study investigates the microwave-assisted synthesis of cobalt (Co) metal-organic frameworks (MOFs), their characterization and application in the adsorption of ciprofloxacin (CPR) and fluoxetine (FLX) from aqueous solutions for removal purposes. The main reagents used were $Co(NO_3)_2 \cdot 6H_2O$ as the metal precursor, terephthalic acid (H_2BDC) as the organic ligand, and dimethylformamide (DMF) as the solvent. The synthesis employed 0.5 mmol of the metal precursor and 1.1 mmol of the ligand, each solubilized in 5 mL of DMF, totaling 10 mL of solution per PFA tube. The Co-MOF microwave-assisted synthesis was carried using a 700 W ramp for 5 minutes, followed by a 250 W hold for 236 minutes with an average temperature of 130 °C. The Field Emission Gun Scanning Electron Microscopy (FEG-SEM) analysis of the Co-MOF revealed a lamellar, plate-like morphology, while Brunauer–Emmett–Teller (BET) analysis indicated a specific surface area of 3.80 m^2/g. Adsorption experiments were conducted using 10 mg of Co-MOF in 50 mL of 10 mg L^{-1} pharmaceutical solutions under 400 rpm agitation, with collecting of 30 to 300 seconds. The maximum adsorption efficiencies of 30.1% were observed for CPR at 240 s and 41.2% for FLX at 300 s. A reversible and dynamic adsorption-desorption behavior was observed, with no clear stabilization within the evaluated time range. The pharmaceutical concentrations were determined by HPLC-RP (A: Aquous - B: Organic, C18 with wavelengths of 278 (CPR) and 224 (FLX)) comparing the samples with a 10 mg L^{-1} blank and using calibration curves of y = 168,367x − 51,130 for CPR and y = 91,042x − 66,057 for FLX, both with R^2 = 0.999. The limits of detection and quantification (LOD/LOQ, mg L^{-1}) were 0.188/0.627 for CPR and 0.153/0.511 for FLX.

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Miniaturized solid-liquid extraction combined with GC×GC-TOFMS for the quantification of NSO-HET markers in Ascidians (Phallusia nigra)

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Palavras Chave:*nitrogen-,sulfur-,and oxygen-containing heterocycles,bidimensional gas chromatography,marine bioindicators*

Highlights

A green miniaturized MSLE–DμSPE combined with GC×GC–TOFMS was developed for the determination of NSO-HET in marine organisms.

Resumo/Abstract

Ascidians are effective bioindicators of marine pollution due to their sessile nature and capacity to bioaccumulate organic contaminants. Nitrogen-, sulfur-, and oxygencontaining heterocycles (NSO-HETs) have received attention as emerging contaminants that serve as sensitive molecular markers of petrogenic inputs. However, their trace-level occurrence and the analytical challenge of simultaneous determination by conventional one-dimensional gas chromatography limit application. In this study, a GC×GC-TOFMS combined with MSLE-DμSPE method was developed to quantify NSO-HETs markers in ascidians. Different GC×GC-TOFMS conditions were tested using 55 NSO-HET standards to achieve the best separation of the target analytes. Ascidian (Phallusia nigra) were collected from Todos os Santos Bay (Brazil) near a floating gas station. Samples were dissected into branchial basket and tunic tissues, lyophilized, and subjected to the MSLE–DμSPE procedure previously developed in our research group, prior to GC×GC– TOFMS analysis under optimized conditions. The method exhibited excellent linearity ($R^2 \geq 0.99$) and suitable sensitivity for trace-level determination, with limits of detection and quantification compatible with the concentrations typically found in marine organisms. The method approach was successfully applied to real samples, enabling the separation of NSO-HET target from aromatic interferences. Benzothiophenes, dibenzothiophenes, carbazoles, and dibenzofurans were observed in the highest concentrations in the branchial basket. This study represents the first application of GC×GC-TOFMS combined with a sustainable, miniaturized extraction strategy for the determination of a large number of petrogenic NSO-HET markers in ascidians, reinforcing the study's potential for advanced environmental monitoring of petrochemical impacts in coastal ecosystems.

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Multielement and bioaccessible contents of edible and medicinal mushrooms using the in vitro INFOGEST Protocol and MIP OES

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Palavras Chave:*Mushrooms,Multielement analysis,INFOGEST 2.0 protocol,MIP OES,Dietary Reference Intake*

Highlights

Combining MIP OES analysis and*in vitro*INFOGEST digestion provides insight into mineral bioaccessibility in mushrooms

Resumo/Abstract

Mushrooms have attracted increasing scientific interest due to their high medicinal and nutritional value. This study examined the multielemental*in vitro*bioaccessibility contents of elements in eleven species of edible and medicinal mushrooms from the Brazilian Atlantic Forest. The study used acid digestion in a closed system and microwave-induced plasma optical emission spectrometry (MIP OES), as well as simulated gastrointestinal digestion according to the*in vitro*INFOGEST 2.0 protocol. After optimization by 2^3 factorial design, the acid digestion method was validated with the variables 2 mL HNO_3 65% (m m^{-1}) + 2 mL H_2O_2 30% (m m^{-1}) + 4 mL H_2O (ultrapure). This method was used to determine the total contents of Ca, Cr, Cu, Fe, K, Mg, Mn, Ni and Zn, as well as the contribution of the bioacessible fraction in relation to the Recommended Dietary Allowances (RDA). The results (in mg kg^{-1}) showed wide variability of elements among the species, with*Favolus brasiliensis*standing out for presenting the maximum values of Ca (4028.26), Cr (2.84), Cu (13.50) and Zn (100.87).*Lentinus berteroi*presented the highest levels of Mg (1722.79) and Mn (24.12), while*Cordyceps sinensis*concentrated the maximum values of Na (819.53) and Ni (3.27). Furthermore,*Lentinus gilbertsonii*and*Oudemansiella cubensis*stood out for its highest Fe (109.72) and K (37,572.4) content, respectively. Accuracy was evaluated through addition and recovery tests. The bioaccessible fraction of the evaluated elements ranged from 11.50 to 85.17%. Although Fe presented high total levels, its bioaccessibility was limited, contributing only 1.3 to 3.0% of the RDA. In contrast, Mn and Cr showed high gastrointestinal release, providing up to 39.4 and 44.3% of the RDA, respectively. Validation of the bioaccessibility test by mass balance indicated recoveries between 80.28 and 125.85%. Therefore, mushrooms have nutritional potential to be used as ingredients in functional foods and mineral supplement.

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NADES: Stability, Extraction Performance, and Compatibility with GFAAS for Potentially Toxic Elements

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Palavras Chave:*Alternative solvents,sample preparation,toxicity,animal tissues,vegetable tissues*

Highlights

NADES enhanced element stabilization at higher temperatures.

NADES remained stable across storage times and conditions.

NADES were compatible with GFAAS for inorganic contaminants determination.

Resumo/Abstract

Sustainable analytical methods that present low toxicity, low cost, and reduced waste generation—both in procedures and supplies—have gained increasing attention in accordance with the principles of Green Chemistry. The growing interest in the application of natural deep eutectic solvents (NADES) is associated with their low toxicity, biodegradability, low cost, water solubility, and minimal waste generation.

The aim of this study was to employ NADES in sample preparation for the quantification of potentially toxic elements (As, Cd, and Pb) by graphite furnace atomic absorption spectrometry (GFAAS) in animal and plant tissue samples. NADES were synthesized from lactic acid (LA), glucose (Glu), choline chloride (ChCl), and citric acid (CA), and used as extraction solvents for inorganic elements. Spectral and non-spectral interferences arising from the sample preparation medium were also evaluated.

Both NADES with a molar proportion of 1:1:10 exhibited suitable characteristics for sample treatment. The obtained viscosity values were comparable to that of water at room temperature (0.976 mPa·s), enabling compatibility with the GFAAS introduction system. Density measurements of the diluted solutions were 1.03 g cm^{-3} for NADES (LA–Glu–W) and 1.01 g cm^{-3} for NADES (CA–ChCl–W). NADES stability was further assessed under two storage conditions—refrigeration and desiccation—over five months. FTIR spectra indicated preservation of the precursor reagents in the synthesized NADES throughout the evaluated period, regardless of storage method.

The VE sample preparation method was very efficient using both NADES (LA-Glu-W and CA-ChCl-W). Synergistic effects between the studied NADES and the chemical modifier $Pd(NO_3)_2$ were observed, mainly for NADES (CA-ChCl-W), which achieved recoveries ranging from 95 to 96% for Cd and Pb in standard reference materials (SRM). This performance can be attributed to the ability of citric acid act as a chemical modifier especially for Pb determination.

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New Analytical Method Based On Free-Solution Capillary Electrophoresis (FSCE) For The Determination Of Glyphosate, Glyphosinate, And AMPA

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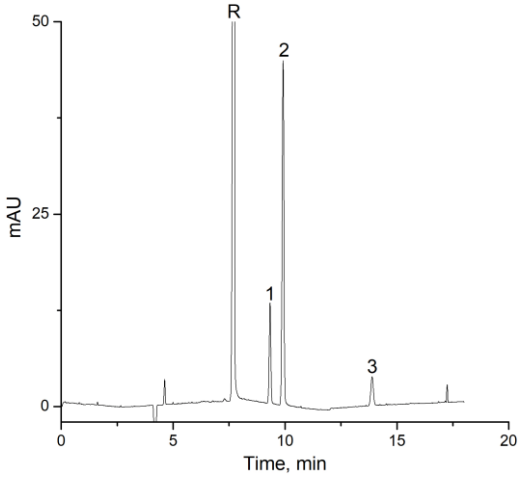
Palavras Chave:*capillary electrophoresis, herbicides, environmental matrices, derivatization,capillary electrophoresis, herbicides, environmental matrices, derivatization*

Highlights

New analytical method for the determination of glyphosate, glyphosinate, and AMPA
Identification and quantification of herbicides in environmental matrices
Capillary electrophoresis and herbicides

Resumo/Abstract

The herbicides glufosinate, glyphosate, and their main metabolite, AMPA, have been widely used in agriculture, and their increasing use has raised concerns about their toxicity. The objective of this study was to develop and validate an analytical method based on free solution capillary electrophoresis (FSCE) with UV detection for the identification and quantification of these compounds in environmental matrices. A derivatization reagent (Dansyl chloride, DNS-Cl) was used to develop the method; the herbicide standards were prepared at 20 mg L-1, and a sodium tetraborate (TBS) buffer at 50 mmol L^{-1} and pH 9.2 was used as the running electrolyte. The instrumental separation conditions were as follows: voltage: 15 kV; temperature: 25°C; injection: 30 mBar x 5 s. The following parameters were tested to optimize the method: reaction time (30, 45, and 66 min), TBS concentration in derivatization (20 and 30 mmol L-1), and pH of the derivatization reaction (10.2, 10.5, and 10.9). The best results (analytical signal) were obtained with a reaction time of 60 min, 20 mmol L-1 of TBS, and pH 10.5. Figure 1 shows the optimized separation system. Since the preliminary results were satisfactory, the next step will be to validate and apply the method to river and potable water, after sample preconcentration.



Herbicides standard mixture (20 mg L-1) R. reagent; 1. Glufosinate; 2. AMPA; and 3. Glyphosate.

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Non-destructive classification of tomato seeds to preserve traditional varieties

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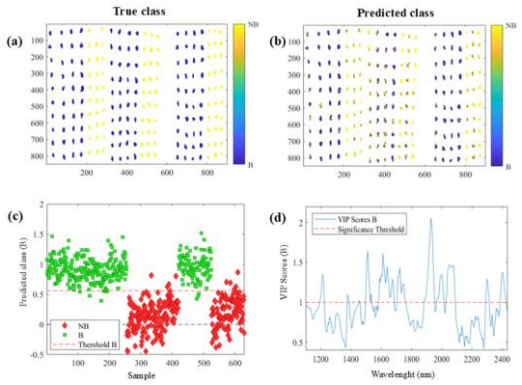
Palavras Chave:*Seeds, Non-destructive analysis, HSI-NIR, PLS-DA*

Highlights

HSI-NIR images for non-destructive analysis of seeds; Identification of traditional varieties; Pixels by pixels vs object level PLS-DA classification models; PLS-DA models with 99.3% accuracy.

Resumo/Abstract

The introduction of improved tomato varieties into agricultural systems to increase productivity has led to severe genetic lost in the crop[1]. Genetic and phenotypic characterization of varieties at the seed level can help to prevent the loss of tomato genetic diversity. Although efficient, techniques such as DNA molecular markers and protein electrophoresis are costly and destructive[2]. Thus, this study developed a rapid, non-destructive method based on hyperspectral imaging in the near-infrared (HSI-NIR) combined with chemometrics to identify and distinguish traditional tomato seed varieties, offering a practical tool for diverse production and research systems. Four varieties of tomato seeds traditionally grown in the Basque Country, Spain, and three non-traditional varieties from the region were obtained commercially. A total of 630 seeds (90 per variety) were analyzed using an HSI-NIR (Specim) system with a spectral range of 996–2505 nm. MATLAB R2015a coupled with HYPER-Tools[3] software was used for the pre-processing and classification steps. Partial least squares discriminant analysis (PLS-DA) models were constructed to distinguish among Basque (B) and non-Basque (NB) varieties. The models for discriminating achieved an accuracy of 84.6% and 99.20% at the pixel and object level, respectively. Subsequently PLS-DA model was constructed to discriminate among the four Basque varieties of seed: Loide (LO), Pikoluze (PI), Deusto (DE) and Aretxabaleta (AR). The pixel-level model showed sensitivities ranging from 0.60 to 1.00 and specificities ranging from 0.88 to 0.99. At the seed level, the respective ranges were 0.87 to 1.00 and 0.89 to 1.00. The spectral regions between 1500 and 1780 nm and around 1900, 2100, 2180, and 2470 nm (Fig. 1d) corroborated the predictive performance of the models. Therefore, the HSI-NIR technique, combined with chemometrics, has demonstrated potential for seed discrimination, representing an advance in the preservation of tomato varieties.



Pixel-based model true class (a) and predicted class (b); Object-based model (c); VIP scores (d)

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One-pot iron determination in fortified flours using Thymol–1,10-phenanthroline deep eutectic solvent and smartphone-based digital image photometry

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Palavras Chave:*In situ complexation,smartphone-based digital image photometry,Green Analytical Chemistry,Microextraction*

Highlights

A thymol/1,10-phenanthroline deep eutectic solvent enabled iron extraction and sensing in fortified flours

Practical and user-friendly approach exploiting smartphone-based digital images

Resumo/Abstract

Iron-enriched flours are an important public health strategy to reduce anemia. The conventional procedures for iron determination in fortified flours generally involve acid digestion followed by determination using flame atomic absorption spectrometry or inductively coupled plasma optical emission spectrometry, which require labor-intensive sample preparation, hazardous reagents, and costly instrumentation. In this context, an analytical method based on the simultaneous analyte extraction and complexation using a deep eutectic solvent (DES) composed of thymol and 1,10-phenanthroline was proposed. The procedure was performed in polypropylene microtubes, yielding a colored DES phase, enabling the smartphone-based colorimetric measurement. The responses at channel B (RGB color system), corresponding to the complementary color of the formed complex, were selected as the analytical parameter. Under optimized conditions (50 µL aqueous Fe(II) solution or 50 mg flour sample, 100 µL DES (0.8:0.2 molar ratio of thymol:1,10-phenanthroline), 200 µL of 2.5% w/v ascorbic acid, and 5 min of reaction under agitation), a linear response was obtained for iron concentrations ranging from 1.5 to 20.0 mg L^{-1}, described by the equation $S = (2.5 \pm 0.1)C + (100 \pm 1)$, $r = 0.997$, where S corresponds to 255 − B. The limit of detection was 0.5 mg kg^{-1} and the coefficient variation was 1.4% (n = 10). Accuracy was assessed by comparing results with a reference procedure based on acid extraction followed by either ultraviolet–visible molecular spectrophotometry or ICP-OES, yielding relative errors of −17.1% to 4.1% and 0% to 18%, respectively. Owing to its simplicity, cost-effectiveness, and alignment with green analytical chemistry principles, the proposed method represents a promising alternative for routine quality control of iron-enriched flours with the perspective of extending the application to other food matrices.

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Optimization of a Disposable Pipette Extraction (DPX) method for fluralaner analysis in bovine plasma by LC-MS/MS

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Palavras Chave:*Fluralaner,LC-MS/MS,Disposable pipette extraction,Multivariate optimization*

Highlights

Fluralaner pharmacokinetics in bovine plasma by LC-MS/MS. DPX as fast and sustainable sample preparation. Optimization of DPX protocol using a Central Composite Design.

Resumo/Abstract

Fluralaner is an ectoparasiticide widely used to control fleas, ticks, and botflies, administered topically. Although its use is well-established in dogs and cats, the recent approval for bovine application demands pharmacokinetic studies. In order to determine the fluralaner plasma concentration curve over time, sensitive and reliable analytical methods have been implemented, such as liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). Considering the complexity of the plasma matrix, a sample preparation step is crucial to avoid analytical problems such as clogging of the system and effects such as carryover. In this sense, this study outlines the development and optimization of a sample preparation method based on disposable pipette extraction (DPX) for determination of fluralaner in plasma samples by LC-MS/MS. Chromatographic separation was achieved using a mobile phase gradient consisting of water (phase A) and methanol (phase B) on a C18 column (2.1 mm × 50 mm, 1.8 µm). Crucial parameters related to DPX protocol were optimized through uni and multivariate approaches. In the evaluation of the DPX extraction phase, commercial phases such as C8, C18, NH2, and hydrophilic-lipophilic balance (HLB) were evaluated, and HLB phase showing the highest extraction efficiency up to 40%. Also, desorption solvent was evaluated, and methanol led to higher recovery. For DPX multivariate optimization, a Central Composite Design (CCD) was applied, evaluating the number of extraction and desorption cycles (3 to 7), and equilibrium time (20 to 60 seconds). CCD demonstrated the influence of each variable on the analyte recovery using the predicted values of desirability, which showed that using 7 extraction cycles, 5 desorption cycles with an equilibrium time of 40 seconds led to higher desirable values. This method was applied in bovine plasma samples, achieving recovery rates over 80%, highlighting the efficiency of the developed method.

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Paper-based analytical devices as alternative platforms for experimental activities in high school chemistry laboratories.

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Palavras Chave:*green chemistry, teaching, microfluidics, paper, titration*

Highlights

Low-cost, disposable, global affordable and equipment free device for chemical education Innovative paper-based methodologies to perform acid-base and precipitation titrations

Resumo/Abstract

µPADs associated with colorimetric detection have attractive features in chemistry due to their small size and portability. These devices have become popular for demonstrating experiments or teaching analytical chemistry for high school students. This study describes the construction of µPADs through stencil printing or wax printing techniques to teach redox reactions, acid-base and precipitation titrations using distance-based measurements. For stencil printing, the layout with a circular zone and two detection zones connected by two microfluidic channels were drawn in Corel Draw. A paper substrate was laminated with a press and a layer of vinyl adhesive was added to it. The paper was cut by a paper cutter and adhesive edges were removed. For proof-of-concept, a redox reaction with sodium hypochlorite (colorless) and N-N diethyl p phenylenediamine(red) generates a purple product. For acid base and precipitation titrations, the devices were wax-printed on paper in a layout with a circular zone connected to a rectangular channel. To perform acid base titrations, the channel was filled with a 0.05 mol L^{-1} NaOH solution with phenolphthalein. Then 4.5 µL of acetylsalicylic acid were added to the circular zone. The length of the discolored zone was measured with a digital caliper. An analytical curve with R^2 = 0.9949 from 5.0 to 16.4 mm when the concentration varied from 0.005 to 0.05 mol/L. For chloride precipitation titration, $AgNO_3$ and K_2CrO_4 were by applying 10 uL of a 0.1 mol/L silver nitrate solution to the zone. 10 uL of potassium chromate was applied to the zone, producing a brick-red Ag_2CrO_4.10 uL of NaCl was applied to the zone. NaCl reacts with silver chromate (brick-red color) to form AgCl (white precipitate). An analytical curve with R^2 = 0.9854 was obtained. It was possible to detect chloride in real samples of different brands of saline solution and olive brine and corn preserve with satisfactory results.

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Performance Evaluation of High-Field Orbitrap and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Complex Matrices

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Palavras Chave:*Complex matrices,Mass Spectrometry,Orbitrap,FT-ICR MS,NSO Compounds*

Highlights

- High Field Orbitrap applied to Complex Matrices

- Multivariate analysis comparative between FT-ICR MS vs High Field Orbitrap

- DBE diagram heatmap

Resumo/Abstract

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is widely regarded as the benchmark technique in petroleomics due to its ultrahigh resolving power and mass accuracy. However, its high acquisition and maintenance costs limit widespread use. High-field Orbitrap (HFO) mass spectrometry has emerged as a promising alternative, although its performance still requires systematic evaluation, particularly for challenging applications such as the molecular characterization of crude oils from different geological origins. In this study, ten crude oil samples from the Brazilian pre-salt province—five marine and five lacustrine, representing two sedimentary basins—were analyzed by ESI(−) FT-ICR MS and ESI(−) HFO MS (resolution: 840,000 at*m/z*400). Molecular formula assignments were grouped into heteroatom classes (NSO), and the data were evaluated using box plots, DBE versus carbon number distributions, and principal component analysis. HFO enabled the assignment of approximately 2,500 molecular formulas, whereas FT-ICR MS assigned around 4,500. Despite this ~45% lower coverage, HFO preserved the overall distribution of major heteroatom classes. Notably, S_1O_4 species—important molecular markers—were detected at relatively higher abundances in HFO data. Both techniques successfully discriminated marine and lacustrine oils based on NSO composition, DBE, and carbon number. Marine samples showed higher oxygen content, DBE, and carbon number, while lacustrine samples exhibited relatively higher nitrogen content. Although HFO presents reduced performance, particularly at higher*m/z*, it provides sufficient resolution and mass accuracy to distinguish crude oils by geochemical origin, supporting its use as a cost-effective alternative for routine petroleomic analyses.

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Planejamento de Experimentos aplicado à hidrólise química da CMS de tilápia: aminoácidos livres e avaliação do grau de hidrólise por OPA e HPLC-FLR.

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Palavras Chave:*DoE, HPLC-FLR, Grau de hidrólise, Aminoácidos livres, Hidrolisado proteico.,DoE,HPLC-FLR,Grau de hidrólise,Aminoácidos livres,Hidrolisado proteico*

Highlights

The DoE the optimization of the chemical hydrolysis of tilapia CMS, maximizing free amino acids in the hydrolyzed fraction and allowing the comparison of the degree of hydrolysis by OPA and HPLC-FLR.

Resumo/Abstract

A indústria de processamento de peixe gera grandes quantidades de resíduos proteicos, que são desperdiçados ou utilizados como coprodutos de baixo valor agregado. A produção de hidrolisados de proteínas de peixe (HPP) representa uma estratégia eficiente para o aproveitamento desses resíduos. Os HPPs correspondem a misturas de aminoácidos, oligopeptídeos e polipeptídeos. Devido à presença de aminoácidos livres, o HPP tem se consolidado como uma tecnologia promissora na agricultura, como um bioinsumo de alto valor agregado. Nesse contexto, este trabalho objetivou aplicar o Planejamento de Experimentos (DoE) à hidrólise química da carne mecanicamente separada (CMS), obtida a partir dos resíduos da filetagem da tilápia-do-Nilo, visando à obtenção de hidrolisados ricos em aminoácidos livres e à avaliação do grau de hidrólise determinado pelos métodos com reagente Ortoftaldeído (OPA) no método espectrofotométrico e por cromatografia líquida de alta eficiência (HPLC) associada ao detector de fluorescência (FLR). Nesta pesquisa foram conduzidos três planejamentos experimentais independentes, utilizando ácido fosfórico, ácido cítrico e hidróxido de potássio. Onde foi empregado um Delineamento Composto Central Rotacional (DCCR) com dois fatores: tempo de reação e concentração do reagente. Os fatores foram avaliados em cinco níveis, compostos por 4 pontos fatoriais; 4 pontos axiais e 5 pontos centrais, utilizados para a estimativa do erro puro e para a verificação da curvatura da superfície de resposta. Dessa forma, cada planejamento envolveu 13 ensaios, realizados de forma aleatorizada, totalizando 39 experimentos. As variáveis resposta incluíram a concentração de aminoácidos livres e o grau de hidrólise (GH%). O estudo possibilitou otimizar a hidrólise química da proteína de peixe e os resultados reforçaram o potencial do HPP como alternativa tecnológica para a valorização de resíduos de peixe na produção de bioinsumos agrícolas.

Agradecimentos/Acknowledgments

FAPEMAT, CAPES, INCT NanoAgro, CNPq, Amaggi e Ambios Agro.

Portable and Benchtop Infrared Spectroscopy for CBD Quantification in Medicinal Cannabis Oils from Brazil and Italy

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Palavras Chave:*Medicinal Cannabis, IR, Cannabinoids, Quantification, Chemometrics.*

Highlights

Infrared spectroscopy combined with chemometrics provides accurate CBD quantification in medicinal*Cannabis*oils from Brazil and Italy using portable and benchtop instruments in diverse oily matrices.

Resumo/Abstract

Medicinal*Cannabis*oils are used in the treatment of refractory epilepsy, with cannabidiol (CBD) contributing to seizure reduction and improved quality of life. In Italy,*Cannabis*products can be purchased in specialized stores without a medical prescription, whereas in Brazil access requires a prescription, and high costs have led families and non-profit associations to produce artisanal oils. Ensuring the quality and cannabinoid content of these oils is essential to guarantee their therapeutic efficacy. This study evaluated infrared (IR) spectroscopy combined with chemometrics for CBD prediction in medicinal*Cannabis*oils from Brazil and Italy, using both portable and benchtop instruments (NIR and MIR regions). Brazilian samples included 69 laboratory-prepared oils with different vehicles (olive, coconut, sunflower, soybean, and MCT oils); reference quantification was performed by HPLC-DAD. Italian data comprised eight commercial oils and their dilutions prepared in olive and MCT oils, resulting in 61 samples. Partial least squares (PLS) regression models were developed separately for each dataset (70% calibration, 30% external validation). The PLS models enabled accurate CBD prediction in both Brazilian and Italian oils (Table 1). Despite differences in concentration ranges, vehicles, brands, and origins, robust models were obtained for both datasets ($R^2 \geq 0.94$ and no significant bias), demonstrating the applicability of IR spectroscopy as a rapid, non-destructive tool for cannabinoid quantification in diverse oily matrices. These results support the potential of IR-based methods for quality control of medicinal*Cannabis*oils.

Dataset	Instrument	CBD Range (% w/w)	Pre-processing	# Latent variables	RMSEP (%)
Brazil	Benchtop MIR	ND – 0.88%	EMSC	7	0.05
	Benchtop NIR			6	0.03
	MicroNIR™			4	0.07
Italy	Benchtop MIR	0.1 – 33.6%	1st Der (SG, 2nd, 31pt)	4	0.71
	Benchtop NIR		EMSC	3	0.62
	MicroNIR™			3	0.61

ND = not detected by the reference method.

Table 1. PLS performance for CBD quantification in Cannabis oils.

Agradecimentos/Acknowledgments

The authors would like to acknowledge Instituto Nacional de Tecnologias Analíticas Avançadas – INCTAA and CNPq. The authors also acknowledge Brazilian non-profit associations for sharing information on medicinal*Cannabis*oil preparation protocols.

Portable biosensor based on urease immobilized in alginate spheres for urea determination by smartphone-based digital image photometry

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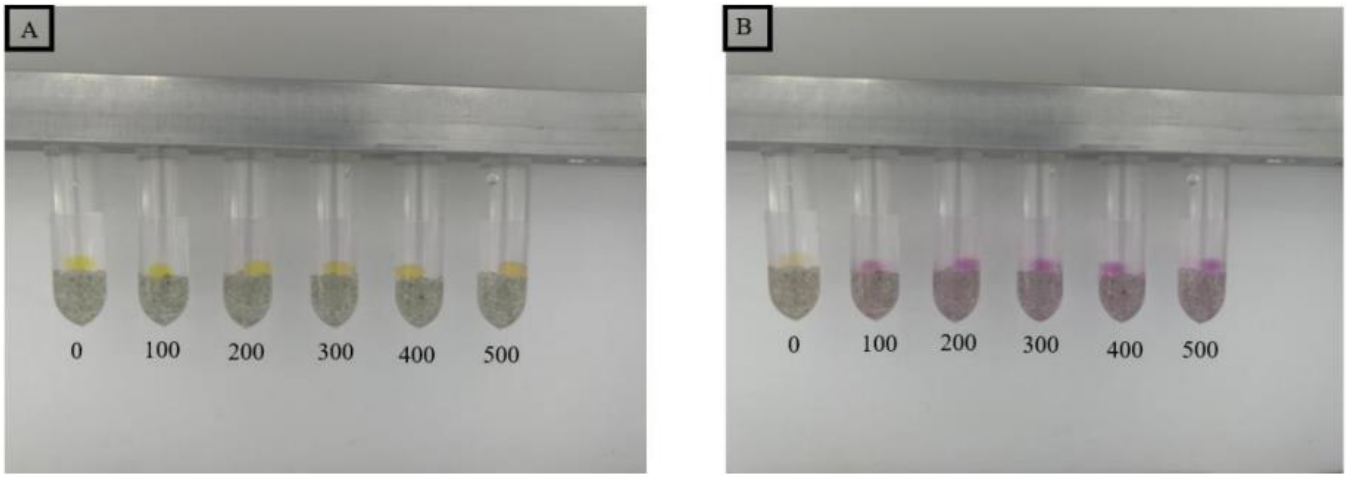
Palavras Chave:*Enzyme immobilization, Food, Urea, Alginate, Colorimetric analysis, Green Analytical Chemistry.*

Highlights

A green biosensor based urease immobilized in alginate beads. Smartphone-based digital image photometry enables in situ analysis. Portable and low-cost platform for urea screening in milk quality.

Resumo/Abstract

Urea determination is relevant for clinical monitoring and food quality control, and a particular application relies on detecting milk adulteration. Usual methods include urease-based enzymatic assays with spectrophotometric readout and automated systems, which provide good analytical performance but generally require specific laboratory infrastructure. This requirement can limit applicability for rapid screening at the sampling site or in scenarios with restricted access to equipment. In this context, this work proposes a sustainable and low-cost optical biosensor for urea quantification, integrating immobilization of urease and phenol red indicator in calcium alginate beads and smartphone-based digital image photometry. The analytical principle relies on urease-catalyzed urea hydrolysis, which generates ammonia and increases the pH within the alginate beads. Ammonia generation shifts phenol red color from yellow to red/pink (pH 6.8–8.4), enabling indirect urea detection. The colorimetric response was monitored by digital videos using a smartphone and processed by digital image analysis to extract RGB values. Channel G was selected for quantification, as it showed the highest sensitivity to chromatic changes associated with phenol red. Under optimized conditions, the method exhibited a linear response in the range of 100–400 mg L^{-1} ($y = 0.000383x - 0.0377$, $R^2 > 0.99$), with a limit of detection of 50 mg L^{-1}. The procedure was applied for determination of urea in milk samples (recoveries > 100%), after protein precipitation using CaCl2. The procedure requires minimal reagents, using 1 mg phenol red, 60 mg of urease, and 100 mg sodium alginate to produce approx. 80 sensing beads, reinforcing its compliance with Green Analytical Chemistry principles. Overall, the proposed strategy shows strong potential for rapid, on-site urea screening, combining simplicity, portability, and low operational cost.



Beads with urea (A) before and (B) after 15 min. Numbers: concentration (mg L^{-1})

Agradecimentos/Acknowledgments

The authors acknowledge CAPES, CNPq, FAPESP, and Fealq for financial support.

Potencial Analítico do Carvão de Casca de Abacaxi com Ag-Nps: Desenvolvimento de Dispositivo Eletroquímico para a Detecção de Íons Chumbo (II)

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Palavras Chave:*Biocarvão,Eletrodos modificados,Ananas comosus,Chumbo (II),Sensores eletroquímicos*

Highlights

Pineapple biochar–AgNP electrode for Pb(II) detection.
Modified electrode boosts Pb(II) preconcentration and voltammetric response.
Low-cost sustainable sensor for Pb(II) monitoring in water.

Resumo/Abstract

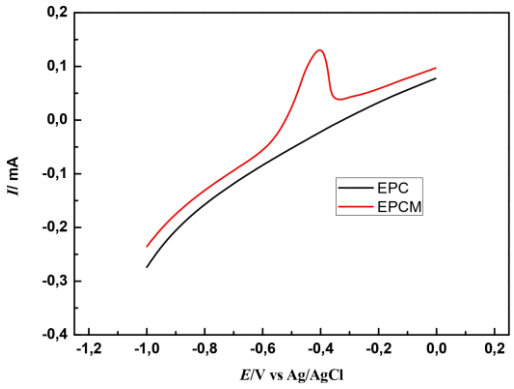
A contaminação ambiental por metais pesados demanda métodos sensíveis, seletivos e de baixo custo para o monitoramento da qualidade da água. Nesse contexto, sensores eletroquímicos modificados com materiais derivados de resíduos agroindustriais têm se destacado como alternativas sustentáveis. Neste trabalho, foi desenvolvido um eletrodo de pasta de carbono modificado com biocarvão obtido da casca de abacaxi (Ananas comosus) incorporado com nanopartículas de prata (EPCM), aplicado à determinação de chumbo(II) em soluções aquosas.

O biocarvão foi obtido por pirólise da biomassa seguida de ativação química e posterior incorporação de nanopartículas de prata, visando aumentar a área superficial, a capacidade adsortiva e a condutividade elétrica do material. O modificador foi incorporado à pasta de carbono em diferentes proporções para avaliar sua influência na resposta eletroanalítica.

As determinações foram realizadas por voltametria de redissolução adsortiva por pulso diferencial utilizando um sistema de três eletrodos. Os eletrodos modificados apresentaram aumento significativo da corrente de pico para Pb^{2+} em comparação ao eletrodo não modificado, indicando maior eficiência na etapa de pré-concentração do analito e melhoria na transferência de carga, atribuídas à presença das nanopartículas de prata e à estrutura porosa do biocarvão.

Os parâmetros experimentais foram otimizados, incluindo pH (5,00), tempo de pré-concentração (1 min) e composição da pasta (20% do modificador). Nas condições otimizadas foi obtida resposta linear na faixa de 5–100 µg L^{-1}, com coeficiente de correlação de 0,99 e desvio padrão relativo inferior a 5%.

Os resultados demonstram que o biocarvão funcionalizado com prata é um modificador promissor para eletrodos voltamétricos sustentáveis, com potencial aplicação no monitoramento ambiental de chumbo em águas.



Voltamogramas de comparação do eletrodo de pasta de carbono não modificado e modificado

Agradecimentos/Acknowledgments

Universidade Estadual de Goiás e Centro de Análises, Inovação e Tecnologia em Ciência Naturais e Aplicadas da UEG – CAiTec. Recurso financeiro proveniente do Edital Pró-Projeto UEG n. 20/2023.

Precipitation titration based on distance measurements in µPads for chloride determination in real samples.

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Palavras Chave:*analytical chemistry, chemical reactions, miniaturization, visual detection, portable instrumentation.*

Highlights

Low-cost, disposable, global affordable and equipment free device for chemical education; An innovative teaching method for visually monitoring precipitation titration.

Resumo/Abstract

Paper-based microfluidic analytical devices with colorimetric detection have proven to be attractive for applications in chemical analysis due to their low cost and accessibility. Distance-based measurements is a simple method for applications in resource-limited laboratories and for teaching analytical chemistry. This study describes the fabrication of µPADs for chloride titration by precipitation using distance-based measurements. The devices were wax-printed on chromatographic paper in a layout with a circular zone with a 5 mm diameter connected to a rectangular channel 40 mm long x 2 mm wide. The titration between silver nitrate and potassium chromate was performed by applying 10 µL of 0.1 mol/L silver nitrate solution to the zone that filled the entire channel. After drying, 10 µL of potassium chromate was applied to the zone, resulting in a brick-red coloration indicating the formation of silver chromate. After drying, 10 µL of sodium chloride was applied to the zone. The NaCl reacts with the silver chromate to form silver chloride which is a white precipitate. The titration process continues as the channel changes color (from brick-red to yellow/white). The length of the discolored channel is measured with a digital caliper or ruler. To obtain the calibration curve, standard sodium chloride (NaCl) solutions with different mass/volume concentrations (0.005 g/mL, 0.01 g/mL, 0.02 g/mL, 0.03 g/mL, 0.04 g/mL, and 0.06 g/mL) were prepared to be applied to the zone of the devices, and solutions of 4% w/v K_2CrO_4 and 0.1 mol/L $AgNO_3$ were prepared. An analytical curve with R^2 = 0.9854 was obtained. Chloride detection was possible in real samples of saline solution and olive brine with satisfactory results. Based on the obtained data, the use of µPADs with distance measurements has offered satisfactory performance for real samples. Distance-based detection titrations have proven to be a low-cost method compared to conventional titrations and shorter analysis times.

Agradecimentos/Acknowledgments

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Preliminary selection of a corn flour matrice for iron and folic acid reference material development

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Palavras Chave:*Reference material,Corn flour,Matrix selection,Food enrichment*

Highlights

Degerminated non-enriched corn flour showed more suitable characteristics for controlled enrichment. First step toward a reference material for iron in enriched corn flour.

Resumo/Abstract

Mandatory enrichment of flours with iron and folic acid in Brazil requires reliable analytical methods and suitable reference materials for quality control. However, the availability of certified reference materials (CRMs) for this matrix is still limited, especially for corn flour. According to USDA, non-enriched degerminated corn flour contains approximately 1.1 mg.100 g^{-1} of iron and negligible folic acid levels, supporting its use as a low-analyte base matrix. In this context, this work aimed to perform a preliminary study for the selection of a candidate matrix for a CRM for iron and folic acid in enriched corn flour, in accordance with ISO 17034.

All experiments were conducted at LACEN/SC, Brazil, under analytical quality control (ISO/IEC 17025), with reference standards and measurement uncertainty evaluation.

Three commercial corn flours with different processing and enrichment characteristics were evaluated: non-enriched whole corn flour (NEWCF), non-enriched degerminated corn flour (NEDCF), and enriched degerminated corn flour (EDCF). Samples were characterized in terms of moisture and volatile matter, titratable acidity, lipids, total iron, pH, and ash content. Analyses were performed in triplicate, and results were expressed as mean ± standard deviation.

Differences in composition were observed among the evaluated matrices, mainly regarding lipid and iron contents. The NEWCF presented higher lipid content, which may compromise its long-term stability. The NEDCF showed lower natural iron content and lower lipid levels, characteristics desirable for a matrix intended for controlled enrichment. The EDCF exhibited higher iron content, reflecting industrial enrichment, and was used only as a compositional reference.

Based on the results, the NEDCF showed more favorable characteristics as a base matrix, mainly due to its lower natural iron and lipid contents, which are desirable for controlled enrichment and further studies.

Corn flour matrix*	Moisture (%)	Titrable acidity	Lipids (%)	Total iron (mg.100g^{-1})	pH	Ash (%)
Whole, unenriched	10.22±0.02	1.79±0.01	4.37±0.05	1.67±0.04	6.28±0.01	1.13±0.01
Degerminated, unenriched	9.46±0.07	0.86±0.02	1.69±0.04	0.69±0.02	6.11±0.02	0.40±0.01
Degerminated, enriched	12.92±0.03	1.12±0.02	1.53±0.15	8.47±0.13	6.13±0.02	0.450±0.002

*Analyses were performed on samples as received.

Table 1 - Preliminary characterization of corn flour matrices candidates

PYROLYSIS OF SUGARCANE BAGASSE AND TEXTILE SLUDGE: A CHEMICAL PERSPECTIVE OVER THE BIO-OIL COMPOSITION

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Palavras Chave:*sugarcane bagasse,textile industry sludge,pyrolysis,bioproducts.*

Highlights

Research into the pyrolysis of sugarcane bagasse and residual textile sludge has shown the generation of bio-oils with a composition rich in high-value-added chemicals.

Resumo/Abstract

Pyrolysis is an efficient thermochemical route for converting biomass into value-added products, primarily bio-oils, which are complex mixtures whose complete characterization poses an analytical challenge. To understand the bio-oils at a molecular level, techniques such as gas chromatography-mass spectrometry (GC-MS) allow the identification of volatile and semi-volatile organic compounds, and ultra high-resolution mass spectrometry (UHRMS) enables advanced chemical characterization and the determination of elemental formulas of the most polar components (Couto et al., 2025). In this context, we conducted a chemical investigation of bio-oils from sugarcane bagasse (SCB) and textile-industry sludge (WST) using microscale pyrolysis at 550 °C. The bio-oils generated were analyzed by GC-MS (Shimadzu Co, model QP2010 SE), and a FT-Orbitrap UHRMS (Thermo Scientific, model Exactive HCD Plus). GC-MS analyses indicated a high production of alcohols and phenolic compounds for both bio-oils, as well as a large number of hydrocarbons for the bio-oil from textile industry wastewater sludge (WST). UHRMS results revealed a predominance of phenolic and aromatic nitrogen compounds, allowing a wide chemical characterization than that by GC-MS. The integrated analytical approach enabled in-depth molecular characterization of the volatile fraction of the bio-oils, thereby contributing to the identification of potential products with higher added value. Overall, preliminary results indicate that bio-oils obtained from SCB and WST have high potential as sources of value-added chemicals from renewable sources.

References:

Couto, A. C. de F.*et al.ACS Measurement Science Au*, v. 5, 2025, p. 687-694.

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Quantificação de arsênio em amostras de insulina por ICP-MS após avaliação de interferência de cloreto.

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Palavras Chave:*Insulina, impurezas elementares, célula de colisão, interferência isobárica.*

Highlights

Accurate quantification of arsenic in insulin samples using ICP-MS with a collision cell to correct isobaric spectral interferences.

Resumo/Abstract

Impurezas elementares podem estar presentes em medicamentos, excipientes ou princípios ativos, introduzidas de forma natural, intencional ou acidental durante as etapas de produção. O arsênio (As) compõe a classe 1 de impurezas elementares na indústria farmacêutica devido ao efeito potencialmente tóxico ao organismo humano. Por serem ubíquos no ambiente, esses elementos devem ser obrigatoriamente monitorados, por critérios estabelecidos pela Farmacopeia dos Estados Unidos (USP). A insulina é um biofármaco utilizado para a manutenção da homeostase glicêmica no tratamento do diabetes mellitus, doença de alta prevalência no Brasil. Por ser uma solução salina, a insulina apresenta altas concentrações de cloreto, principalmente como cloreto de zinco. Ao ser nebulizada pelo sistema de introdução do espectrômetro de massas com plasma indutivamente acoplado (ICP-MS), tendo argônio como gás de purga, a solução pode estar sujeita a interferência isobárica na quantificação de As, um elemento monoisotópico. Para avaliar a interferência, foram realizados ensaios de adição e recuperação de As nas concentrações de 1, 5 e 10 µg/L, na presença de cloreto variando de 50 a 1000 ppb, com e sem o uso de célula de colisão. O limite de detecção e o limite de quantificação para As foram de 0,053 µg/L e 0,178 µg/L, respectivamente, com recuperações entre 80,7% e 94,5%. A quantificação de arsênio foi aplicada a amostras de insulina regular e NPH, cujos resultados permaneceram abaixo do limite máximo permitido pela USP para medicamentos injetáveis (15 µg/dia). A maior concentração média de As foi observada em amostras de insulina regular (6,43 µg/L). Não foi observada interferência significativa do cloreto nas condições avaliadas. Os resultados demonstram que o método é adequado para o monitoramento de As em amostras de insulina, com valores em conformidade com os limites regulatórios.

Agradecimentos/Acknowledgments

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Laboratório de Química Analítica Instrumental e Ciências Forenses (LaQAFor)

Rapid fractionation of crude petroleum oil (SARA) for characterization of saturated and aromatic biomarkers using GC×GC-TOFMS

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Palavras Chave:*Petroleum,Sample preparation,SARA,GC×GC,Mass Spectrometry*

Highlights

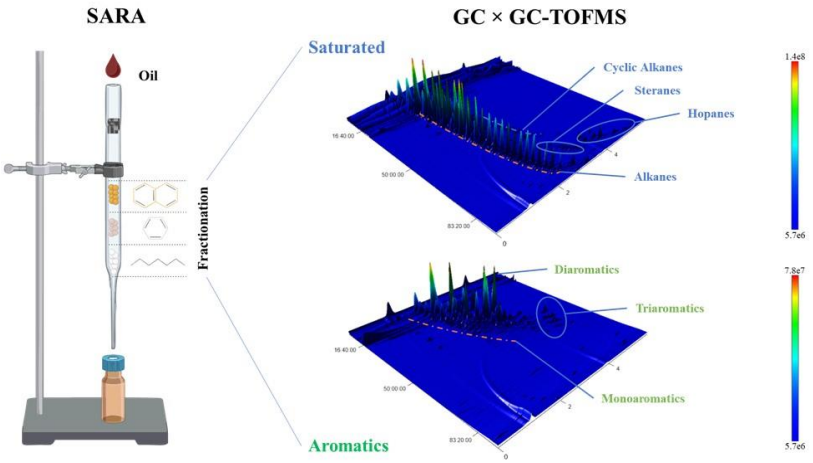
Simple, rapid, and cost-effective SARA adaptation using open-column chromatography;

Efficient SARA adaptation with low cross-contamination;

Reliable biomarker identification via GC×GC-TOFMS.

Resumo/Abstract

Crude oil is a complex mixture of compounds, and fractionation is essential for the detailed characterization of biomarkers. The SARA method, widely used for compositional analysis of crude oil, separates samples into saturated hydrocarbons, aromatic hydrocarbons, resins, and asphaltenes. The saturated and aromatic fractions contain crucial information for assessing the oil's thermal maturity, degradation, and origin. Conventional SARA protocols frequently suffer from cross-contamination between fractions, and few studies report solutions to this problem. We propose an adaptation of the SARA method that improves separation efficiency while maintaining low cost and simplicity. Using approximately 12 mg of sample, with minimal handling and only two mobile phases in a simple open-column setup, we fractionated saturated and aromatic compounds. Comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry (GC×GC-TOFMS) was then used for compound identification. The results demonstrated rapid and efficient fractionation, with low cross-contamination (2.1% aromatics in the saturated fraction; 0.7% saturated compounds in the aromatic fraction), well below the 10% reported in the literature. A total of 392 compounds were identified (242 in the saturated fraction and 150 in the aromatic fraction). Important biomarkers, including hopanes, steranes, diamonoids, and various aromatic compounds, were identified, validating the analytical approach. Overall, the method is fast and economical, and it preserves chemical information during fractionation, making it suitable for the analysis of saturated and aromatic hydrocarbons.



Graphical Abstract

Agradecimentos/Acknowledgments

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Reanalyzing Public Metabolomics Data Uncovers N-Acyl Lipid Dysregulation in Atopic Dermatitis

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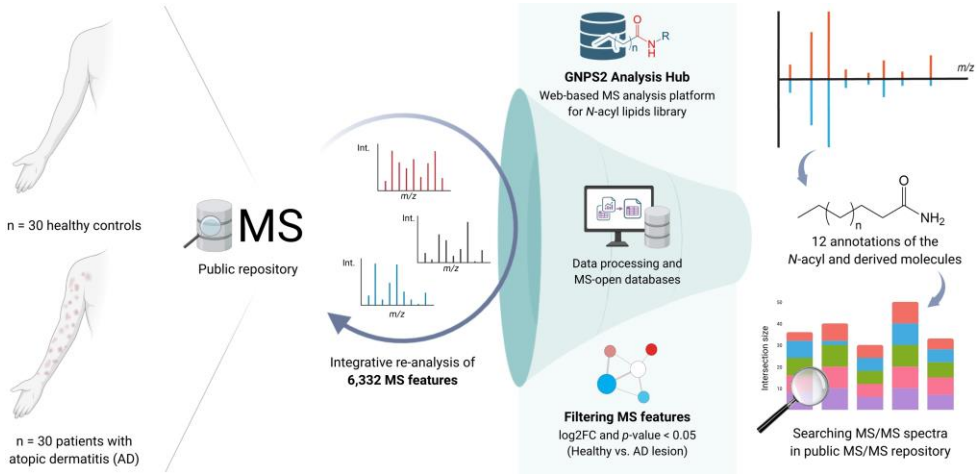
Palavras Chave:*Atopic dermatitis,N-acyl lipids,metabolomics,exposomics,GNPS2.*

Highlights

Public LC-MS/MS human skin metabolomics data uncover overlooked N-acyl lipids and derivatives dysregulation in atopic dermatitis.

Resumo/Abstract

Atopic dermatitis (AD) is a chronic inflammatory skin disease characterized by epidermal barrier dysfunction and alterations in lipid metabolism. Although previous metabolomics studies have elucidated the main classes of lipids involved in skin physiology, the role of*N*-acyl lipids and derivatives in AD remains poorly understood. Thus, we performed a reanalysis of a public dataset[1] of LC-MS/MS-based metabolomics from skin swabs of healthy patients (n = 30) and patients with atopic dermatitis (n = 30). A total of 6,332 MS features (defined by*m/z*and retention time) were evaluated using statistical criteria (fold change ≥ 2 and*p*-value < 0.05), enabling the mapping of molecular differences between healthy and AD skin. All features were queried against public MS/MS spectral libraries using the GNPS2 Analysis Hub[2], resulting in the annotation of*N*-acyl lipids and structurally related molecules. Among the detected features, 102 showed significant alterations in AD samples, including 12 annotated metabolites belonging to three subclasses: (1)*N*-acylethanolamines and long-chain amides, (2) carnitines, and (3)*N*-acyl amino acids, dipeptides, and derivatives. To further contextualize these findings, fastMASST searches revealed that several of these metabolites are widely detected in microbial and personal care product datasets, offering a potential context for the microbiome and exposome that explains their presence in skin affected by atopic dermatitis. Taken together, these findings reveal a distinct and class-specific signature of*N*-acyl lipids, carnitines, and amino acids/dipeptides associated with dysregulation in atopic dermatitis, thus demonstrating the power of reanalyzing public data to uncover overlooked biochemical patterns associated with skin barrier dysfunction.



Overview of the reanalysis of public LC-MS/MS-based metabolomics data in atopic dermatitis.

Agradecimentos/Acknowledgments

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Reversible Microfluidic Platform for Spheroid Culturing, Downstream Characterization, and Dynamic Anticancer Susceptibility Testing

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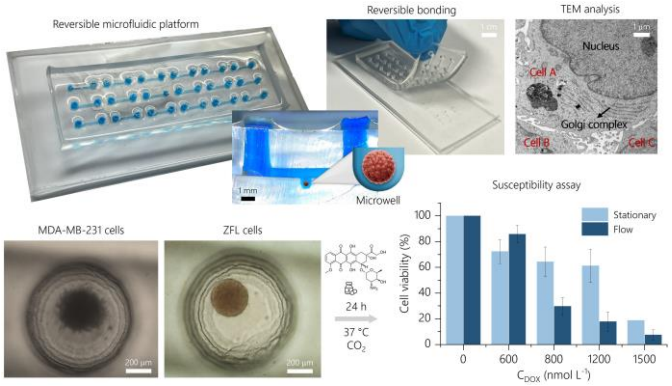
Palavras Chave:*Standardized microfluidic protocol,3D spheroid culture,Reversible bonding strategy,Dynamic perfusion,Drug susceptibility testing*

Highlights

Reversible PDMS microfluidic platform enables standardized spheroid culture, intact recovery and physiologically relevant drug testing under dynamic flow.

Resumo/Abstract

Three-dimensional (3D) spheroid cultures have emerged as advanced in vitro models that better recapitulate the physiological complexity of native tissues than conventional two-dimensional systems; however, their broader adoption is limited by the lack of standardized protocols, limited access to downstream analyses, and the predominance of static culture conditions. Here, we present a standardized microfluidic protocol for reproducible spheroid formation, maintenance, and handling using a microwell-based platform. The workflow addresses operational challenges such as bubble management, surface passivation, medium exchange, and flow control, enabling both static and dynamic operation modes with controlled perfusion at physiologically relevant conditions. The device was fabricated by low-cost replica molding using 3D-printed masters produced by stereolithography. The resulting microfluidic channels presented cross-sectional dimensions of approximately 840×940 µm (height × width), while the microwells exhibited 840 µm diameter. It was assembled through a reversible bonding strategy ensuring leak-free operation while allowing straightforward disassembly for intact spheroid recovery. Uniform spheroids were generated from human breast cancer cells and zebrafish liver cells, demonstrating protocol robustness across biological models. Reversible assembly enabled gentle spheroid retrieval and ultrastructural analysis by transmission electron microscopy, revealing preserved cellular organization and metabolic activity. Dynamic susceptibility assays under continuous perfusion showed enhanced cytotoxic response to doxorubicin compared to static exposure, highlighting the importance of physiologically relevant mass transport in 3D drug screening. Overall, this work provides an accessible microfluidic framework integrating reproducible 3D culture, reversible assembly and dynamic perfusion, improving the physiological relevance of in vitro pharmacological and toxicological assays.



Reversible microfluidic platform for 3D spheroid culture and improved drug response under flow.

Agradecimentos/Acknowledgments

The authors acknowledge Angelo L. Gobbi, Maria H. O. Piazzetta and Rui C. Murer for helping with the microfabrication processes.

rGO/AgNPs nanocomposite applied to the determination of Cu(II) and Mn(II) ions in water by LIBS

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Palavras Chave:*LIBS; rGO/AgNPs nanocomposite; signal intensification; metal ions; water analysis.*

Highlights

rGO/AgNPs nanocomposite as an emission signal enhancer in LIBS. Increase of LIBS signals of Cu(II) and Mn(II) ions of 14x and 4x, respectively. Feasible strategy to improve detectability in LIBS.

Resumo/Abstract

One of the limitations of LIBS (Laser-Induced Breakdown Spectroscopy) is its poor detectability, especially in the analysis of liquid samples. The present work aims at evaluating whether a solid substrate consisting of reduced graphene oxide nanocomposite deposition decorated with silver nanoparticles (rGO/AgNPs) can be used as a signal intensifier in LIBS for the determination of Cu(II) and Mn(II) ions in water. The LIBS system consisted of a pulsed Nd:YAG laser (5 ns, 90 mJ, 20 Hz) operating at 1064 nm. The nanocomposite was synthesized from graphene oxide and silver nitrate (1:5 m/m ratio) and reduced with sodium borohydride using the Liquid-Liquid Interfacial Route. Subsequently, 3.0 mL of the rGO/AgNPs suspension was deposited on water contained in a beaker. A filter paper ring was fixed on a dip-coater holder, which was immersed into the beaker and then removed, forming a nanocomposite film on the paper surface. The nanocomposite was characterized by Raman spectroscopy and Scanning Electron Microscopy (SEM). In Raman spectrum, D and G bands were observed, with an increase in intensity mainly in the D band, facilitating the anchoring of AgNP. SEM images showed AgNP clusters superimposed on rGO and covering the cellulose fibers. For LIBS determination, 600 µL of water sample (n=3) wase deposited on the ring, which was dried in an oven (60 °C for 2 h). The nanocomposite proved to be viable for the determination of Cu(II) and Mn(II) ions in water, providing emission signals approximately 14 and 4 times higher than those obtained with the deposition of the solution on filter paper alone. Linear responses up to 0.5 mg L^{-1} were obtained, with R^2 of 0.95 and 0.99, allowing detection limits (3·sb/slope) of 3.0 µg L^{-1} and 9.0 µg L^{-1} for Cu(II) and Mn(II) ions, respectively. Recoveries from 60 to 120% and from 80 to 95% were obtained for Mn(II) and Cu(II) ions, respectively, as a consequence of matrix effects.

Agradecimentos/Acknowledgments

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Screening of Metals from E-Waste Via Energy-Dispersive X-Ray Fluorescence (EDXRF): Analytical Approaches Based on Chemometric Fingerprinting

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Palavras Chave:*EDXRF,Cooper,Chemometrics,PCBs,Green Chemistry*

Highlights

Green analytical strategy: direct analysis of solids by EDXRF without reagent consumption; Efficient temporal discrimination of smartphones (2002–2020) based on chemical fingerprinting.

Resumo/Abstract

Introduction: Characterization of PCBs from e-waste is vital for recycling planning [1]. Traditional quantification involves laborious preparation; conversely, Energy-Dispersive X-ray Fluorescence (EDXRF) offers a high-throughput Green Chemistry approach [2]. This study employed EDXRF fingerprinting and chemometrics to evaluate the metallic evolution of smartphones (2002–2020).**Methodology:**1.9 kg of PCBs from end-of-life smartphones were disassembled and milled (<53 μm). Spectra were acquired using a benchtop EDXRF (Rigaku NEX QC+, Ag tube, SDD). Three instrumental conditions were applied [3], and the data were processed in MATLAB®.**Results:**Pearson correlation analysis showed high covariance among the 21 samples, justifying the use of multivariate methods. Principal Component Analysis (PCA) explained 98.65% of the variance. PC1 (94.06%) revealed a clear separation in PCB composition: positive loadings were dominated by Cu (Kα, Kβ) lines, while negative loadings were characterized by Zn (Kα) and Sn (Kα), reflecting variations in the conductive base-to-solder ratio. The score plots indicated manufacturing alterations. PC2 (3.61%) and PC3 (0.98%) elucidated residual interfaces: PC2 highlighted Fe, Ni, and Ag, while PC3 identified environmental markers such as Pb and As, indicating fluctuations aligned with RoHS guidelines.**Conclusion:**The approach validated EDXRF-chemometrics for e-waste characterization, distinguishing samples temporally and highlighting the persistence of Cu and transitions in solders (Zn, Sn). This strategy assists urban waste sorting, aligning with Circular Economy principles.
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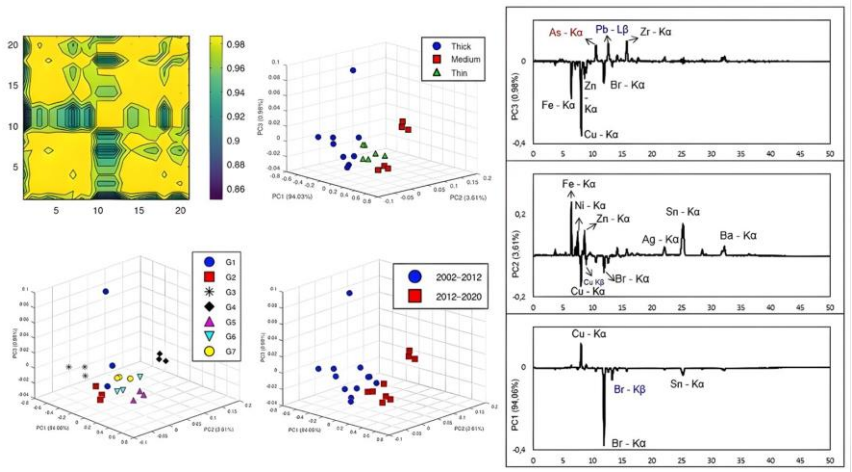


Fig. 1: Chemometric fingerprinting of PCB samples from different periods via EDXRF spectra.

Agradecimentos/Acknowledgments

São Paulo Research Foundation (FAPESP), Brazil. Processes Numbers #2024/17925-1, #2019/01102-8, #2025/19876-0, and #2025/16683-7, National Council for Scientific and Technological Development (CNPq) grant no. 302085/2022, and CAPES - Finance Code 001

Selective leaching and separation of rare earth elements from discarded neodymium–iron–boron magnets

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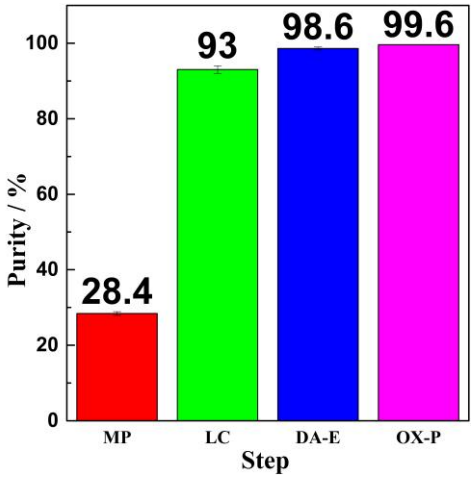
Palavras Chave:*Rare earth elements, Hydrometallurgy, Liquid–liquid extraction, Decanoic acid, Electronic waste.*

Highlights

Selective recovery of rare earth elements from NdFeB magnets using mild hydrometallurgical conditions; Low co-dissolution of Fe and Ni enables high-purity separation of Nd, Pr, and Dy.

Resumo/Abstract

The recovery of rare earth elements (REEs) such as Nd, Pr, and Dy from neodymium–iron–boron (NdFeB) magnets has emerged as a focus as a sustainable alternative to address the limitations and complexity of ore processing. The main challenge in magnet recycling is separating REEs from the concomitant elements (iron, cobalt, nickel, and boron). In this context, this work aims to recover REEs from NdFeB magnets in three steps: selective leaching, liquid–liquid extraction, and precipitation. Leaching of the magnet powder (MP) was conducted for 720 min at 79 °C, using a solid–liquid ratio of 0.05 g mL^{-1} and levulinic acid at 1.7 mol L^{-1}. The leaching efficiencies for Nd, Pr, Dy, B, Co, Ni, and Fe were 84, 82, 86, 74, 66, 0.4, and 0.7 %, respectively. Thus, it was possible, already in the leaching step, to separate Ni and Fe from the other elements. Proceeding to REE extraction, the leachate (LC) was mixed with decanoic acid at a molar fraction of 0.2:0.8, respectively. Extraction was performed at 60 °C for 30 min, yielding extraction efficiencies of 68, 69, and 75 % for Nd, Pr, and Dy, respectively. The remaining elements stayed in the aqueous phase, thereby enabling the separation of cobalt and boron. Finally, the decanoic acid-rich phase (DA-E), enriched in REEs, was mixed with various oxalic acid solutions to promote back-extraction and simultaneous precipitation of the REEs as oxalates. Solutions of 0.55 and 1.1 mol L^{-1} were evaluated. Using the 0.55 mol L^{-1} solution, the recovery of Nd, Pr, and Dy was 90 % for Nd and Pr, and 33 % for Dy. When employing the 1.1 mol L^{-1} solution, the recovery increased to 98 % for Nd and Pr, and 66 % for Dy. Figure 1 shows the evolution of REE purity relative to the contaminants throughout the three steps. Mixed-REE oxalate (OX-P) was obtained with 99 % purity. This work demonstrates the feasibility of recovering high-purity REEs under less environmentally and human health-harmful conditions.



Purity of REEs across process steps. MP: powder, LC: leaching, AD-E: extration, OX-P: precipitation.

Agradecimentos/Acknowledgments

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Sensores eletroquímicos baseados em biocatalisadores miméticos à base de carboximetilcelulose funcionalizada para detecção de organofosforados

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Palavras Chave:*enzymeless,Hidrogel,eletrodo impresso,Paraoxon-metil,Pesticida Organofosforado*

Highlights

Plataforma eletroquímica descartável e biomimética baseada em gel de CMC–imidazol para detecção rápida e*in situ*de pesticidas organofosforados.

Resumo/Abstract

Os pesticidas organofosforados constituem um grupo notável de contaminantes químicos de interesse ambiental, devido à sua elevada toxicidade e ampla aplicação agrícola. Nesse contexto, sensores eletroquímicos descartáveis surgem como alternativa para detecção rápida, de baixo custo e*in situ*desses compostos. Este trabalho propõe o desenvolvimento de uma plataforma de sensoriamento eletroquímica baseada na funcionalização da carboximetilcelulose (CMC) com grupos imidazol (API), projetada como mimetizador enzimático das enzimas fosfotriesterase ou fosfatase alcalina.

A síntese da CMC funcionalizada foi realizada por reação de acoplamento, seguindo metodologias descritas por Takarada et al. [1]. Inicialmente, 0,125 g de CMC foram dissolvidos em 17,5 mL de água deionizada sob agitação overnight. A ativação dos grupos carboxílicos ocorreu em banho de gelo pela adição de 5,925 mmol de EDC e de NHS, seguida da inserção de 0,7 mL de 1-(3-aminopropil)imidazol (API). O anel imidazol atua como centro nucleofílico, favorecendo a catálise da hidrólise do paraoxon-metil.

A caracterização por FTIR revelou, para a CMC, banda larga entre 3600–3200 cm^{-1} atribuída ao estiramento O–H, com sobreposição de bandas de amida, e sinal em ~1600 cm^{-1} associado ao grupo carboxilato. Na CMC funcionalizada observaram-se bandas em ~1550 cm^{-1}, atribuída ao C=N do anel imidazólico, e em ~1670 cm^{-1}, relacionada à deformação N–H, indicando modificação do polímero.Os dados de titulação potenciométrica corroboraram a funcionalização do material devido à variação do pKa para cada material.

Estudos eletroquímicos serão conduzidos em eletrólito de suporte (tampão BR), utilizando Voltametria Cíclica (VC) e Voltametria de Onda Quadrada (VOQ), na presença e ausência do analito, visando avaliar a influência do pH e do tempo de incubação na resposta eletroquímica do sistema CMC–imidazol frente ao paraoxon-metil.

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CNPq, Processo número 403306/2023-0

FAPEG

Universidade Federal de Goiás (UFG)

CAPES

Simultaneous and individual determination of Brilliant Blue FCF and Tartrazine dyes in beverages using smartphone-based digital image analysis

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Palavras Chave:*RGB,Artificial dye,DIA,Green analytical chemistry,Quantification*

Highlights

Digital image analysis complies with the principles of Green Analytical Chemistry;
Twenty samples of different brands of drink flavors were quantified;

Resumo/Abstract

The use of artificial colorants such as Brilliant Blue FCF (E133) and Tartrazine Yellow (E102), either individually or in combination in beverages, may cause adverse effects when safety limits are exceeded, including allergic and anaphylactic reactions. This underscores the need for strict monitoring. In this study, two analytical methods were developed by optimizing the UV-Vis molecular absorption spectrophotometry method, and smartphone-based digital image method (DIA). The latter is rapid, low-cost, and enables in situ analysis. Both methods were validated over the linear range of $1.00x10^{-4}$ to $9.90x10^{-3}$ mg mL^{-1} and applied to quantify E133 and E102 in alcoholic and non-alcoholic beverages, either as single dyes or in mixtures. Both methods exhibited excellent linearity (R^2>0.999), adequate recovery (within the acceptable guideline range), and compliance with homoscedasticity and residual normality criteria. All concentrations measured were below the maximum limits established by Anvisa[1] and the Codex General Standard for Food Additives[2] (<2.0×10^{-1} mg mL^{-1} in alcoholic beverages and <1.0×10^{-1} mg mL^{-1} in non-alcoholic beverages). The DIA method enabled data acquisition and processing in only 3 min, demonstrating efficiency, environmental sustainability, and applicability for in situ monitoring using a smartphone. These findings highlight its potential for routine beverage quality control in line with the principles of green analytical chemistry (GAC).

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Agradecimentos/Acknowledgments

FACEPE, CAPES, LABMAQ/UFRPE, NUQAAPE

Spatial detection of lipids and TCA-cycle metabolites in breast cancer biopsies by DESI mass spectrometry imaging after combined training

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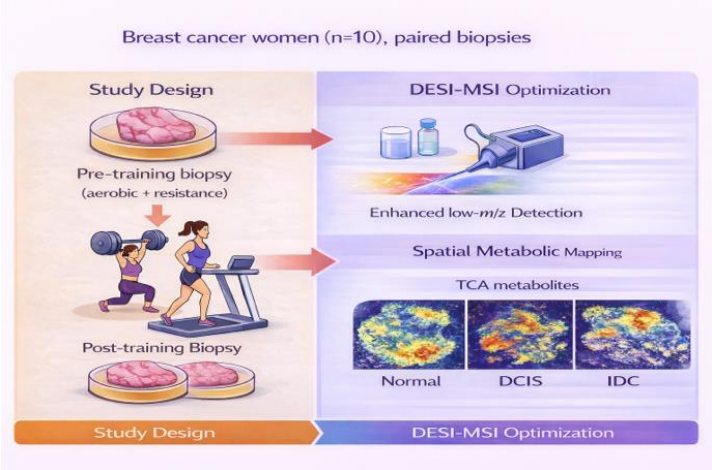
Palavras Chave:*breast cancer,mass spectrometry imaging,DESI-MSI,spatial metabolomics,combined training*

Highlights

DESI-MSI tuned for low-*m/z*TCA metabolites in breast cancer biopsies
Citrate, oxaloacetate, and α-ketoglutarate mapped in tumor tissue
Metabolites/lipids compared across normal, IDC, and DCIS regions

Resumo/Abstract

Breast cancer is the most incident malignancy and leading cause of cancer death among women in Brazil and worldwide, with marked metabolic heterogeneity. While DESI-MSI excels at lipid imaging, sensitive detection of low-mass metabolites (e.g., TCA intermediates) remains challenging. Here we aimed (i) to optimize DESI-MSI for TCA-cycle metabolites and (ii) to evaluate the feasibility of spatially detecting lipids and TCA intermediates in breast cancer biopsies collected before and after a combined-training (CT) intervention. Tumor biopsy fragments from 10 treatment-naïve women with stage I–III breast cancer were collected pre- and post-chronic CT (≥6 sessions). Starting from lipid-oriented DESI settings and leveraging recent methodological advances, we optimized spray-solvent composition, additive use, spray flow, and capillary voltage to enhance low-*m/z*performance. The optimized conditions yielded higher-intensity low-mass spectra with reduced chemical interference, enabling chemical images that highlight ions of interest. Under these conditions, citrate, oxaloacetate, and α-ketoglutarate were detected and mapped within tissue sections. Spatial profiles were evaluated against histological annotations of invasive ductal carcinoma (IDC), ductal carcinoma in situ (DCIS), and adjacent normal regions, revealing region-dependent signal patterns across malignant and non-malignant areas. These results support DESI-MSI as a label-free platform for in situ investigation of tumor metabolism and provide a practical workflow to extend DESI-MSI beyond lipid-dominant readouts toward small-metabolite imaging in exercise-oncology studies.



DESI-MSI spatial mapping of TCA metabolites in paired breast cancer biopsies pre- and post-training

Agradecimentos/Acknowledgments

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Spatial Metabolomics Reveals Hippocampal Localization of Cannabidiol and Its Metabolites in Mouse Brain

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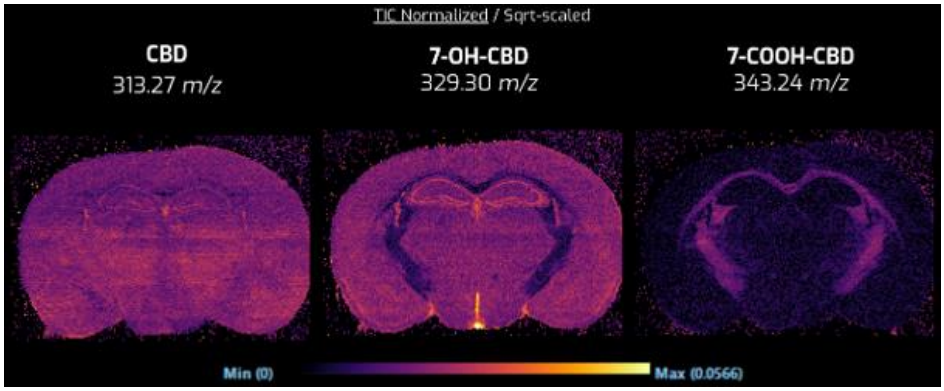
Palavras Chave:*Cannabidiol,DESI-MSI,Mouse brain,Imaging Mass Spectrometry,neurodistribution*

Highlights

DESI-MSI mapped CBD, 7-OH-CBD, 7-COOH-CBD, and CBG in mouse brain after acute dosing. The neurodistribution of the compounds showed a prominent hippocampal localization associated with epileptogenesis.

Resumo/Abstract

Pharmaceutical cannabidiol (CBD) is approved for specific seizure indications, and together with cannabigerol (CBG), it has been investigated as a potential therapy for epilepsy. However, its spatial disposition within the brain remains incompletely understood. In this study, desorption electrospray ionization mass spectrometry imaging (DESI-MSI) was employed to investigate the regional brain distribution of CBD, its major metabolites, and CBG, following acute administration in mice. Male C57BL/6J mice (n = 6; CEUA #6492-1/2024, UNICAMP) received vehicle, CBD, or CBG (100 mg/kg, i.p.) and were euthanized 1 h (CBD) or 2 h (CBG) post-dose. Brain tissues were cryosectioned (20 µm) and analyzed by DESI-MSI in negative ion mode with 50 µm spatial resolution. Compound detection was achieved by monitoring deprotonated precursor ions, revealing well-defined signals for CBD (*m/z*313.217) and its active metabolite 7-hydroxy-CBD (*m/z*329.212), both exhibiting preferential localization in hippocampal regions. In contrast, the inactive metabolite 7-carboxy-CBD (*m/z*343.192) displayed reduced hippocampal signal intensity and a more prominent distribution in regions associated with neuronal connectivity. CBG (*m/z*315.232) was detected at lower intensity and showed a comparatively homogeneous spatial distribution across brain sections. Molecular assignments were supported by high mass accuracy and confirmed by on-tissue MS/MS using analytical standards. These findings demonstrate that CBD and structurally related cannabinoids exhibit distinct regional brain distributions that are not predictable solely from their chemical similarity. DESI-MSI provides a powerful, label-free approach to resolve neuroanatomical localization of cannabinoids, supporting mechanistic studies in cannabinoid pharmacology and toxicology beyond bulk tissue measurements.



DESI-MSI image of cannabidiol and its metabolites in mouse brain tissue after acute administration

Agradecimentos/Acknowledgments

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Spectrophotometric determination of total oil and grease in offshore produced water using synthetic oily water standards: a study of pre-salt oils

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Palavras Chave:*Pre-salt crude oils,Offshore produced water,Total oil and grease,Spectrophotometric method,Synthetic oily water standards*

Highlights

Synthetic oily-water standards replicate Brazilian pre-salt produced water for TOG calibration. Real-sample validation confirms accuracy and precision for low-cost UV-Vis offshore monitoring.

Resumo/Abstract

The determination of Total Oil and Grease (TOG) in offshore produced water is essential for environmental monitoring and regulatory compliance in oil and gas operations. Several methods are used for TOG assessment, including gravimetry, infrared spectroscopy, fluorimetry, GC-FID, TOC analysis, and UV–Vis spectrophotometry. Among these, spectrophotometric approaches stand out for their operational simplicity, relatively low cost, and suitability for routine offshore analysis.[1] However, the complex composition of produced water, including surfactants, corrosion inhibitors, and emulsifying agents, affects analytical performance. Thus, method optimization and validation are required. In this work, a UV–Vis spectrophotometric method was optimized and validated using laboratory-prepared synthetic oily-water standards to simulate offshore produced water conditions. Synthetic standards were prepared following the method of Brant*et al*. (2023)[2] to suit this study. For the three evaluated pre-salt oils, calibration curves from 15 to 125 ppm showed excellent linearity ($R^2 > 0.999$) and high sensitivity, with limits of detection of 1.0–3.0 ppm and limits of quantification of 3.2–9.0 ppm. Precision and accuracy were evaluated using synthetic standards and real produced water samples yielding acceptable relative standard deviations and recoveries of 80–120%. Comparative analysis across the three oils demonstrated consistent performance, indicating negligible matrix effects on TOG quantification. Validation with real produced water further confirmed the method's robustness and repeatability. Overall, the results show that the proposed UV–Vis method is reliable and suitable for routine TOG determination in offshore produced water across multiple pre-salt oil matrices.

Agradecimentos/Acknowledgments

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Spectroscopic Properties of Substituted Phenethylamines: A computational Chemistry and Data Science Approach.

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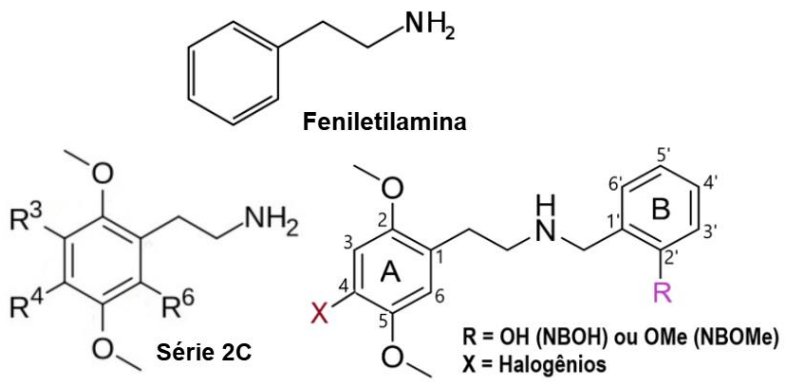
Palavras Chave:*New Psychoactive Substances, Substituted Phenethylamines, Infrared Spectroscopy, Machine Learning, Supervised Classification.*

Highlights

IR spectroscopy classified NBOH, NBOMe and 2C compounds. Spectral databases evaluated with machine learning. Multiclass models showed low error rates.

Resumo/Abstract

New Psychoactive Substances (NPS) have been rapidly introduced into the illicit market, hindering their identification and monitoring. Among them, are the substituted phenethylamines from the NBOH, NBOMe, and 2C series, exhibiting small structural modifications compared to the base structure of phenethylamine. These modifications result in psychedelic effects similar to LSD, but with higher potency at lower doses. The characterization of these substances is commonly performed using Category A analytical techniques, according to the SWGDRUG classification, such as infrared spectroscopy, which allows structural elucidation through the interaction of infrared radiation with molecular vibrational modes. However, despite its high reliability, this method presents limitations related to instrumental cost, sample preparation, and the need for specialized analysts. In this context,*in silico*methods and data science techniques emerge as complementary alternatives for rapid information acquisition. In this study, the functionality of infrared spectroscopy databases for NBOH, NBOMe, and 2C substances, obtained from SWGDRUG and ENFSI, was evaluated using supervised classification models implemented with the PyCaret library. This framework employs multiple algorithms, allowing the selection of the best-performing model and performance assessment through confusion matrix analysis. A multiclass classification approach was applied, without and with mean-centered preprocessing. The best multiclass classification model without preprocessing was Logistic Regression (LR), with an error rate of 5.88%. For the classification with preprocessing the best model was Support Vector Machine with linear kernel (SVM), showing an error of 3.92%. Thus, concluded that the model still requires adjustment, but shows a tendency in separating the molecules and indicates that evaluated infrared spectroscopy libraries are suitable for application in machine learning methods aimed at NPS classification.



Chemical structure of phenethylamine molecules and their derivatives: NBOH, NBOMe and 2C series.

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Statistical Analysis of Synthesis Condition Variations of Sulfur Mustard

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Palavras Chave:*Sulfur Mustard,Multivariate Statistics,Clandestine Synthesis,Chemical Weapons*

Highlights

Deconvolution splits GC–MS overlaps.
Models recover spectra; library IDs.
Impurity fingerprints trace routes.
Evidence for defense and sovereignty.

Resumo/Abstract

This work proposes an analytical workflow to investigate sulfur mustard synthesis using gas chromatography–mass spectrometry (GC–MS) combined with multivariate statistical deconvolution. Bench-scale reactions were performed based on three literature-reported synthetic routes for sulfur mustard production from thiodiglycol using different chlorinating agents (HCl, PCl_3 and $SOCl_2$). Reaction conditions were systematically varied to generate representative datasets of reaction products, residual reagents, and by-products. In total, 48 samples were prepared and analyzed.

GC–MS analyses were carried out using an Agilent 7890A gas chromatograph coupled to a 5975C mass spectrometer equipped with an HP-5MS capillary column. The mass spectrometer operated in electron ionization mode (EI, 70 eV), scanning a mass range from m/z 35 to 500, with chromatographic runs of 35 minutes. The chromatographic data were preprocessed using baseline correction, retention time alignment, and data matrix organization prior to chemometric analysis.

Signal deconvolution was performed using Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) implemented in the MCR-ALS GUI developed by the University of Barcelona. The number of components was estimated using singular value decomposition (SVD), and the iterative optimization was initialized using evolving factor analysis (EFA). Non-negativity and unimodality constraints were applied during model optimization.

The model enabled the resolution of overlapping chromatographic signals and the recovery of spectral and elution profiles of relevant compounds. Among the resolved components, sulfur mustard, oxathiane, and sesquimustard were identified through comparison with the NIST mass spectral library. The proposed workflow demonstrates the potential of chemometric deconvolution to recover chemically meaningful information from complex GC–MS datasets obtained from controlled synthesis experiments.

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Study of Organic Acids Profile in Human Urine by Capillary Zone Electrophoresis Aiming at the Diagnosis of COVID-19

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Palavras Chave:*urine, capillary zone electrophoresis, target metabolomics, machine learning classification, COVID-19*

Highlights

CZE-UV applied to urinary metabolites analysis

Multivariate analysis of electropherograms data

Organic acids profile

Resumo/Abstract

The coronavirus disease (COVID-19) pandemic revealed the need for alternative diagnostic strategies based on accessible and non-invasive analytical approaches. In this proof-of-concept study, the applicability of capillary zone electrophoresis with indirect ultraviolet detection (CZE-UV) was evaluated for the exploratory analysis of four urinary metabolite profiles (tartrate, malate, lactate, and succinate) in samples collected from individuals tested by reverse transcription polymerase chain reaction for severe acute respiratory syndrome coronavirus 2. The electropherogram profiles were pre-processed, and machine learning approaches were applied to classify COVID-19 positive and negative samples. The evaluated models included partial least squares discriminant analysis (PLS-DA), soft independent modeling of class analogy (SIMCA), decision tree, random forest, bagged decision trees, and stochastic gradient descent (SGD). Univariate analysis revealed no statistically significant differences between groups, within 95% confidence interval, indicating substantial overlap in metabolic profiles. Multivariate analysis showed moderate model performance, with limited discrimination by PLS-DA, high sensitivity but low specificity for SIMCA, and balanced yet low overall accuracy for tree-based models. The SGD classifier achieved the best performance, reaching 70% accuracy and a Matthews correlation coefficient of 0.41. Overall, the results indicate that urinary organic acid profiles exhibit limited discriminative power for COVID-19 classification. Nevertheless, this study reinforces the feasibility of integrating CZE-UV with machine learning as an exploratory, low-cost, and non-invasive approach, with potential applications in metabolomics studies and preliminary screening strategies.

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Sustainable solid–liquid microextraction for quantification of alkylated PAHs in sediments impacted by different anthropogenic sources

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Palavras Chave:*APAHs,gas chromatography,green method*

Highlights

A sustainable UAE-MSD was optimized for APAH determination in sediments. Clean-up steps were eliminated, simplifying sample preparation, and method greenness was evaluated using analytical metrics.

Resumo/Abstract

Alkylated Polycyclic aromatic hydrocarbons (APAHs) contamination of sediments through petroleum spills, discharges, and seepages is a widespread environmental problem. In petroleum-derived mixtures, alkylated polycyclic aromatic hydrocarbons (APAHs) often exceed parent PAHs in both concentration and toxicity to aquatic biota. These observations, together with increasing regulatory pressure, highlight the need for effective strategies for APAH determination in environmental matrices. Therefore, this study aimed to optimize a sustainable ultrasound-assisted extraction microscale device (UAE-MSD) method for the determination of 23 APAHs in sediments and to evaluate their potential as markers for different anthropogenic sources. The method proved to be efficient, requiring 25 mg of sediment, 500 µL of dichloromethane:hexane (1:1, v:v) and 23 min of extraction. The UAE-MSD does not require purification steps, thereby reducing sample preparation time. Analyses were performed by gas chromatography coupled to mass spectrometry in selected ion monitoring mode. Evaluation of the UAEMSD method using metrics demonstrated its sustainable potential. Under optimized conditions, the method demonstrated satisfactory linearity (0.25-40 µg L^{-1}; R^2 ³0.99), with detection limit ranging from 1.8 ng g^{-1} (3-MPhen) to 15.9 ng g^{-1} (1-EtNap) and the quantification limit from 6 ng g^{-1} to 53.4 ng g^{-1} for the same compounds (1-EtNap). Correlation coefficients (R2)³ 0.99 were obtained for all compounds. The mean recovery for most of APAHs ranged from 50 to 120% with intraday and interday <20%. The UAE-MSD was applied to 32 sediment samples collected from areas under distinct anthropogenic influences, and APAHs were quantified at concentrations ranging from 6.44 ng g^{-1} (2-MNap) to 986,81 ng g^{-1} (3,6-DMPhen). The highest APAHs concentrations were observed in sites associated with petrogenic sources, characterized by elevated 1-EtNap, 2,6/2,7-DMNap, 2-MAnt,

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Synthesis and application of an eco-friendly nanomaterial for magnetic solid-phase microextraction and determination of Pb in tattoo inks by GF AAS

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Palavras Chave:*Preconcentration,contaminants,new materials,adsorption*

Highlights

Eco-friendly iron oxide nanomaterial from açaí waste was applied in magnetic microextraction.

Slurry sampling GFAAS to determine Pb in tattoo inks was carried out.

Resumo/Abstract

The increasing popularity of tattooing raises concerns about toxic elements in tattoo inks, whose determination remains challenging due to sample preparation and low concentration levels. Therefore, this work aimed to synthetize and apply an eco-friendly iron oxide nanomaterial for the magnetic solid phase microextraction and determination of Pb in tattoo ink samples using slurry sampling in a Graphite Furnace Atomic Absorption Spectrometry (GFAAS). Iron oxide nanomaterial were synthetized using açaí agro-industrial waste and characterized by X-ray diffraction, thermogravimetry and Fourier Transform Infrared Spectroscopy. The nanoparticles were used as sorbent to the dispersive magnetic microextraction. An amount of 400 mg of each sample of tattoo ink was subjected to microwave-assisted acid digestion using 7.0 mL of HNO_3 (≈14 mol L^{-1}) and 1.0 mL H_2O_2 (≈9 mol L^{-1}) and 1.0 mL of ultrapure water. The digested samples were analyzed by Inductively Coupled Plasma Optical Emission Spectrometry (ICPOES) to determine the major composition of the solutions. The levels of the factors pH, mass of nanoparticle and stirring time were optimized using central composite design for the magnetic solid phase microextraction. According to Shapiro-Wilk test, the residues followed a normal distribution. The optimal condition of preconcentration was achieved at pH 11, 24.0 mg of nanomaterial, 120 min of stirring time. Using slurry sampling GFAAS with 500 µL of HNO^3 (≈0.21 mol L^{-1}), the pyrolysis and atomization temperatures were optimized to 800 ºC and 1400 ºC, respectively. The analytical method achieved a limit of detection in aqueous solutions and simulated matrix of 0.2 ng g^{-1} and 0.7 ng g^{-1} of Pb. The determination of Pb in three samples presented

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Synthesis and Characterization of Co(II) and Er(III) MOFs by Microwave Energy: Atenolol Adsorption Study in Aqueous medium

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Palavras Chave:*MOFs,emergent contaminants,Atenolol,microwave synthesis,adsorption.*

Highlights

Microwave synthesis results on a homogeneous material and a faster process

Drug have been accumulating at rivers due to human action

MOF are potential materials to CE adsorption

Resumo/Abstract

Emerging contaminants (ECs) are unmonitored substances that are being extensively researched due to their impacts on ecosystems. Since pharmaceuticals, hormones, cosmetics, and other ECs are present in domestic wastewater, methods for quantifying and remediating these contaminants are being developed. The objectives of this work are the synthesis, characterization, and application of metal-organic frameworks (MOFs) with d-block (Co) and f-block (Er) metals, obtained by the microwave-assisted solvothermal (MW) method, for the adsorption removal of the beta-blocker Atenolol (ATL), widely used in medical treatments. The MOFs were obtained from the reaction of 1 mmol of terephthalic acid (H2BDC), 10 mL of dimethylformamide (DMF), and 0.5 mmol of precursor salts of Co(II) and Er(III), respectively. The reactions were conducted in an MW Mars 6 reactor using power control at a temperature of 160°C. The MOF-Co and MOF-Er samples were characterized by SEM-FEG, where a nanoplatelet morphology was observed in MOF-Co and rods-shaped in MOF-Er, whose surface areas obtained by BET were 3.8 $m^2.g^{-1}$ and 2.0 $m^2.g^{-1}$, respectively. The quantification by reverse phase HPLC(Solvents: A-formic acid 0.001% v/v - B - MetOH, C18 - 15cm, 224nm, retention time 6,9 min) in the ATL adsorption studies was performed using the linear equation obtained using concentration points between 1.0 and 20 $mg.L^{-1}$: $y = 27.206x + 0.280$, $R^2 = 0.997$ and LOD/LOQ (0.016/0.054)$mg.L^{-1}$. Preliminary adsorption tests were performed at 25°C under magnetic stirring at 400 rpm, using 10 mg of each MOF for 50 mL of a 10 $mg.L^{-1}$ ATL solution, collecting aliquots at times between 0.5 and 5 minutes. As a result, 10% adsorption was obtained for MOF-Co and 15% for MOF-Er, both reaching adsorption equilibrium in 2 minutes. Therefore, a good adsorptive capacity of the studied MOFs for ATL was observed, indicating that the materials obtained by MW in a short period of time are promising for the removal of this EC in aqueous medium.

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Synthesis and Characterization of Erbium Metal-Organic Frameworks for Diclofenac and Fluoxetine Adsorption

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Palavras Chave:*Synthesis,Characterization,Adsorption,Drug Metal-Organic Framework.,Drug*

Highlights

Emerging Energies;

Microwave radiation (MW);

Synthesis and Characterization of Metal-Organic Frameworks (MOFs);

Study of drug Adsorption using Er-MOFs;

Resumo/Abstract

This work aimed to explore more efficient energies, such as microwave energy (MW), in the synthesis of Erbium (Er) metal-organic framework (MOF) materials, seeking to obtain a more homogeneous material with greater control over particle size and structure, for the study of drug adsorption, such as Diclofenac (DIC) and Fluoxetine (FLX) in aqueous solution. For the synthesis, terephthalic acid (H2BDC) was used as a ligand and dimethylformamide (DMF) as a solvent. The procedure, using the Mars6 instrument (CEM Corporation), consisted of dissolving 0.5 mmol of the precursor salt and 1.0 mmol of the ligand in 10 mL of solvent under an ultrasonic bath for 20 min. Subsequently, the mixture was transferred to 75 mL PFA tubes and subjected to MW with a 5 min ramp (700 W), followed by a 236 min dwell (250 W) at 160 °C. The materials were characterized: morphological analysis by Field Emission Scanning Electron Microscopy (FE-SEM) indicated rod-shaped structures; surface area analysis using the Brunauer-Emmett-Teller (BET) model showed 1.96 m^2/g. Preliminary adsorption tests were conducted with 10 mg of material in 50 mL of drug solution at a concentration of 10 mg L^{-1} with agitation at 400 rpm, with collection for 30 to 300 seconds. Adsorption studies using the Er-MOF showed values of 15% (DLC) and 20% (FLX). Quantification was performed by HPLC (Phase A: 0.001% formic acid and B: MetOH, gradient, in C18 with wavelengths of 275 (DIC) and 224 (FLX))using the following calibration curve (y = 78.173x + 6.517) for DLC with R^2 of 0.999 and LOD/LOQ (mg L-1) of 0.182/0.608; (y = 91.042x – 66.057) and for FLX with R^2 of 0.999 and LOD/LOQ (mg L-1) of 0.154/0.511 and (y = 166.662x – 8.122). Preliminary results confirm the efficiency of the microwave method in obtaining rod morphology and adsorption ranges between 10-20%.

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Synthesis and evaluation of nitrogen-doped carbon quantum dots as fluorescent probes for Hg(II)detection

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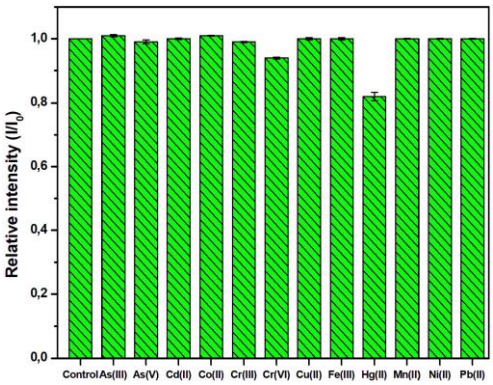
Palavras Chave:*Carbon Quantum Dots,fluorescence,metal ions,Hg(II),fluorescence quenching.*

Highlights

N-CQDs were synthesized by a microwave-assisted method, exhibiting intense blue emission and high responsiveness to the presence of Hg(II), indicating promising potential as fluorescent probes.

Resumo/Abstract

Water and food contamination by metal ions represents a major socioeconomic concern, since several of these species, such as Pb(II), Cd(II), and Hg(II), are toxic even at low concentrations and can cause serious damage to human health and ecosystems. In this context, the development of analytical techniques capable of identifying and quantifying toxic metal ions in different matrices has become increasingly important. Among the available methodologies, fluorescence analysis stands out due to its high sensitivity, operational simplicity, and relatively low cost compared to other analytical techniques.
Carbon Quantum Dots (CQDs) are nanomaterials that have attracted considerable attention as analytical probes, since their fluorescence intensity can vary as a function of analyte concentration. Based on this property, the present work reports the synthesis of nitrogen-doped Carbon Quantum Dots (NCQDs) and their application for the detection of toxic metal ions. The NCQDs were synthesized using citric acid and ethylenediamine as precursors through a microwave-assisted hydrothermal method, without a purification step. The particles exhibited intense blue emission at 440 nm under excitation at 347 nm. Fluorescence experiments were carried out at pH 7 using phosphate buffer, NCQDs at a concentration of 0.1% (v/v), and different metal ions at 1 mg L−1. Under these conditions, only Hg(II) caused a significant fluorescence quenching of 18% (Figure 1). When the probe concentration was reduced to 0.0125% (v/v), fluorescence quenching increased significantly to 52%. In addition, fluorescence quenching showed a proportional relationship with mercury ion concentration in the range of 0.02 to 2.5 mg L−1. Considering the optical properties of the synthesized NCQDs and the preliminary fluorescence quenching studies induced by Hg(II), the proposed material shows great potential for the detection of this metal in aqueous solutions.



Fluorescence of NCQD at 0.1 %(v/v) in the presence of metal ions.

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Technological variability in archaeological ceramics from the São Lourenço Stream (Piauí, Brazil) investigated by pXRF, XRD and PCA

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Palavras Chave:*Archaeometry, Archaeological ceramics, Portable X-ray fluorescence, X-ray diffraction, Multivariate analysis*

Highlights

Archaeometric analyses revealed technological variability in archaeological ceramics, indicating different raw materials and firing conditions across the studied samples.

Resumo/Abstract

Archaeometry provides an interdisciplinary framework to investigate technological choices and cultural practices through the physicochemical analysis of archaeological materials. This study aimed to characterize archaeological ceramics and lithic artifacts from the São Lourenço Stream (Piauí, Brazil) and the Canaã site (Bahia, Brazil), as well as a contemporary ceramic sample, in order to evaluate compositional variability and technological patterns. A total of 46 samples were analyzed using portable X-ray fluorescence (pXRF), X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive spectroscopy (SEM–EDS), and multivariate statistical analysis (PCA and HCA). pXRF data revealed major and trace elements such as Si, Al, Fe, K, Ca, Ti, Mn, Sr, and Zr, allowing the discrimination of lithic materials and distinct ceramic groups associated with each archaeological context. Ceramics from the Canaã site exhibited elevated P_2O_5 contents, consistent with funerary use described for the Aratu Tradition. XRD identified mineral phases including quartz, anorthite, hematite, and microcline, suggesting firing temperatures between 650 and 850 °C in open firing structures. SEM–EDS analyses indicated differences in porosity, temper integration, and sintering degree, reinforcing technological heterogeneity within the ceramic assemblage. A glazed ceramic fragment enriched in Pb and Co was identified, suggesting a historical artifact related to European ceramic production. Multivariate analyses highlighted subgroups reflecting variations in raw material selection, temper addition, and firing conditions. Overall, the results indicate a shared technological background combined with significant variability, suggesting the coexistence of multiple production practices or workshops. This study demonstrates the relevance of integrated archaeometric approaches for understanding technological diversity in archaeological ceramics from Northeastern Brazil.

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The use of deep eutectic solvents as a green chemistry approach in coffee bean sample preparation for multielemental determination

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Palavras Chave:*solventes eutéticos,extração assistida por ultrassom,nutrientes no café,ICP*

Highlights

Evaluate eutectic solvents in coffee sample preparation for multielemental determination

Characterization of eutectic solvents by FTIR-ATR

UAE as a green alternative in coffee sample preparation

Resumo/Abstract

The Coffee fruit comes from Rubiaceae family,*Coffea*genus, which comprises more than 25 species, with*C. arabica*and*C. canephora*being the most commercially significant. During the cultivation phase, parameters such as altitude, soil quality and bean origin (*C. arabica*or*C. canephora*), among others, are monitored (Gonzalez-Rios et al., 2007; Somporn et al., 2011). Determination of macronutrients and micronutrients is also important due to the fundamental role in development of the coffee plant and fruit café (Da Silva, 2009; Ferrão et al., 2017). Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) are used for elemental determination, however, samples must be in a liquid state to application in these techniques. Usually, Microwave-assisted digestion (MW-AD) methods are used for sample preparation. Nevertheless, the use of concentrated acids such as nitric acid (HNO_3), chloridric acid (HCl) or fluoridric acid (HF) turns the procedure environmentally aggressive. In view of this, the present study aimed to evaluate the use of Deep Eutectic Solvents (DES) and ultrasound-assited extraction (UAE) as a green alternative in sample preparation for multielement determination in coffee beans. First, the formation of the citric acid, malic acid and water (Ct:Ma:Wa) solvent in a 1:1:30 molar ratio, respectively, was verified by FTIR-ATR. Subsequently, ICP-OES analysis determined Ca (0,730,73±0,39) mg g^{-1}, K (16,34±1,55) mg g^{-1} and Mg (0,49±0,39) mg g^{-1}, with RSDs of 53%, 9% and 34%, respectively.

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Tunable Polymeric Hybrid Luminescent Sensors from Functionalized BODIPY Derivatives and Lanthanide Complexes toward Multimodal Applications

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Palavras Chave:*BODIPY,lanthanide,fluorescent probe,polymers,luminescent solar concentrator*

Highlights

BODIPY- and lanthanide-doped polymeric films presented a ratiometric temperature sensing (233–393 K), excitation-dependent color for LSCs, and efficient ammonia detection in solid and aqueous media.

Resumo/Abstract

The development of optical sensor platforms has received increasing attention due to the demand for selective and sensitive methods for detecting analytes of biological and environmental relevance. In this context, systems with tunable luminescent responses enable the sensing of various analytes and temperature, while also functioning as photonic devices, such as luminescent solar concentrators (LSCs).[1,2] This work reports PMMA films doped with BODIPY derivatives and Ln^{3+}-complexes, including Eu^{3+}, Tb^{3+}, and Yb^{3+}, obtaining tunable emission properties. In particular, PMMA films doped with BODIPY (0.01 wt.%) and Eu^{3+} complex (2 wt.%) exhibited excitation wavelength-dependent emission, shifting from red (Eu^{3+}, $^5D_0 \rightarrow {}^7F_n$) to green (BODIPY, $S_1 \rightarrow S_0$) as the excitation wavelength varied from 300 to 500 nm. The intrinsic Eu^{3+} quantum yield ranged from 52 to 58%, with excited-state lifetimes of 8.87 – 12.29 ns (BODIPY) and 0.46 – 0.48 ms (Eu^{3+}), suggesting intermolecular energy transfer. Thermometric studies in the 233-393 K range (λ_{ex} = 410 nm) showed a ratiometric response with a maximum thermal sensitivity of 3.60%.K^{-1} at 393 K. Morfological and optical characterization were performed using FTIR, SEM, and emission spectroscopy under solar irradiation. Se-BODIPY-doped films were applied for ammonia detection in aqueous media. The analyses were performed using a smartphone to record RGB parameters inside a controlled illumination box. Tunable emission colors were observed depending on the BODIPY/Ln^{3+} ratio and it indicates the potential applications in luminescent solar concentrators and smart window technologies.[3]

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Untargeted LC-MS-based metabolomic profiling of DMT and 5-MeO-DMT in cell models of neurodegeneration

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Palavras Chave:*Metabolomics,DMT,5-MeO-DMT,neurodegeneration models,LC-MS*

Highlights

Untargeted LC-MS-based metabolomics aims to elucidate the cellular responses and molecular mechanisms of action of DMT and 5-MeO-DMT at sub-toxic concentrations in*in vitro*neurodegeneration models.

Resumo/Abstract

In recent years, psychoactive compounds have garnered significant scientific interest as alternative therapies for neurodegenerative diseases and complex neuropsychiatric disorders, owing to their neuroprotective potential and neuroplasticity-inducing capabilities. N,N-Dimethyltryptamine (DMT) and 5-methoxy-N,N-dimethyltryptamine (5-MeO-DMT) are natural indole alkaloids that exhibit high structural similarity to essential biomolecules in human metabolism, such as the neurotransmitter serotonin. This structural analogy facilitates interaction with 5-HT1A and 5-HT2A receptors, modulating metabolic pathways and cellular signaling processes. However, despite these similarities, these compounds produce distinct actions and subjective effects in humans, and the molecular mechanisms underlying these effects remain to be fully elucidated at the cellular level.

In this context, the present study aims to investigate the metabolic alterations induced by DMT and 5-MeO-DMT in human neuroblastoma (SH-SY5Y) and glioblastoma (U-87MG) cell lines, representing neuronal and glial models, respectively. Preliminary cytotoxicity assays using the resazurin method were conducted for both cell lines across concentration ranges of 0.39-50 µM for DMT and 0.35-45 µM for 5-MeO-DMT, following 24 h of exposure. The results demonstrated no significant changes in cell viability compared to the control group, indicating an absence of acute toxicity at these concentrations. These findings are fundamental for defining a functional concentration capable of inducing cellular signaling without triggering oxidative stress, thereby enabling subsequent untargeted metabolomics assays using liquid chromatography coupled to mass spectrometry (LC-MS). The results are expected to contribute to the understanding of the molecular mechanisms involved in the action of these psychedelics, supporting their translational potential for clinical studies and the development of novel therapeutic strategies.

Agradecimentos/Acknowledgments

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Use of eutectic solvent (ES) to leach metals from nickel-metal hydride battery gridwaste

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Palavras Chave:*Nickel-metal hydride batteries, Hydrophilic eutectic solvents, Metal recovery, Leaching kinetics, Choline chloride,Nickel-metal hydride batteries,Hydrophilic eutectic solvents,Metal recovery,Leaching kinetics,Choline chloride*

Highlights

Kinetic study of Ni and Fe leaching from Fe–Ni grids of spent NiMH batteries using a deep eutectic solvent.

Resumo/Abstract

Nickel-metal hydride batteries utilize a current collector grid composed of approximately 98 % (m/m) iron and 2 % (m/m) nickel. Traditionally, recycling routes for collectors are based on pyrometallurgical processes, which operate at high temperatures and CO_2 emissions, or hydrometallurgical processes, which employ environmentally impactful acids with high operational risks, such as H_2SO_4, HCl, and H_3PO_4. In this scenario, hydrophilic eutectic solvents ($ES_{ph}i$) emerge as a sustainable alternative for selective leaching and metal recovery from metallic alloys. The present study investigated the leaching of Ni and Fe from discarded NiMH battery grids using an $ES_{ph}i$ composed of choline chloride and methanesulfonic acid (ChCl:MSA, 1:1) with 30 % water. The assays were conducted at a solid-liquid ratio of 1:25, evaluating the influence of time (1 min to 12 h) and temperature (40, 60, and 80 °C) on the leaching process. The results demonstrate that higher temperature reduces viscosity, thereby increasing diffusion and interaction between the solvent and the residue.; therefore, for nickel, there was an increase from 20 to 99 % when raising the temperature from 40 to 80 °C. For iron, the maximum leaching efficiency of 98 % was reached in only 180 min at 80 °C. While at 40 °C, only 80 % iron leaching efficiency was obtained after 720 min, the model that best fit the data was the film diffusion model for both Iron and Nickel, indicating that the ES interacts with the waste by diffusion, which is favored by the increase in temperature. Thermodynamic adjustments indicated that $Ea_{(Ni)}$ is 61.1 kJ mol^{-1} and $Ea_{(Fe)}$ is 33.9 kJ mol^{-1}. Thus, optimization yields a temperature of 80 °C and a leaching time of 3 h, resulting in extractions of 99 and 98 % for Ni and Fe, respectively. The ChCl:MSA system demonstrates high efficacy, making it a promising, low-impact route for treating battery waste.

Agradecimentos/Acknowledgments

The authors are grateful to**CAPES**,**CNPq**, and**FAPEMIG**for the support provided during the development of this study.

Uso de solventes eutéticos profundos no preparo de amostras de ração para cães visando à extração de elementos metálicos: um estudo preliminar

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Palavras Chave:*Alimentos para cães,Solventes eutéticos profundos (DES),Determinação de elementos metálicos,ICP OES,Química Analítica Verde*

Highlights

Deep eutectic solvents applied to dog food sample preparation. Green alternative to conventional acid digestion. Preliminary results consistent with label-declared mineral levels.

Resumo/Abstract

O controle de qualidade de rações para cães é fundamental para garantir a adequada ingestão de nutrientes essenciais e a segurança alimentar dos animais. Com o aumento da preocupação dos tutores em relação à alimentação dos pets e a crescente industrialização desse setor, torna-se indispensável o desenvolvimento de metodologias analíticas confiáveis e sustentáveis para a avaliação da composição nutricional desses produtos.

Neste contexto, o presente trabalho teve como objetivo avaliar o uso de solventes eutéticos profundos (DES) como alternativa verde à digestão ácida convencional no preparo de amostras de ração para a determinação de elementos metálicos essenciais. Foram testados três DES à base de cloreto de colina e diferentes ácidos carboxílicos (ácido málico, cítrico e tartárico). Os solventes foram aplicados na extração de Ca, Cu, Fe, K, Mg, Mn e Zn de uma amostra comercial de ração para cães previamente moída, a qual foi submetida à extração em banho ultrassônico a 60 °C por 30 min, utilizando 1 g de solvente. As determinações foram realizadas por ICP OES.

Os resultados obtidos, ainda que preliminares, indicaram que a eficiência de extração dos elementos metálicos variou de acordo com a composição do solvente eutético utilizado. O DES composto por cloreto de colina e ácido cítrico apresentou desempenho ligeiramente superior para a maioria dos elementos avaliados, especialmente Ca, K e Mg. De modo geral, Ca e K apresentaram as maiores concentrações na amostra avaliada (~12 g/kg e ~5 g/kg), enquanto Mg foi observado em concentrações intermediárias (~0,9 g/kg) e os elementos-traço em níveis significativamente inferiores (~16-115 mg/kg), em concordância com valores declarados pelo fabricante.

Os resultados indicam o potencial dos solventes eutéticos profundos como alternativa sustentável para o preparo de amostras em análises de rações para cães, alinhando-se aos princípios da Química Analítica Verde e fornecendo subsídios para estudos futuros.

Agradecimentos/Acknowledgments

As autoras agradecem à Universidade Federal de Ouro Preto pelo apoio institucional e à infraestrutura dos laboratórios utilizados. Agradece ao CNPq e à FAPEMIG pelo incentivo e fomento à pesquisa científica.

Validation of a method using LC-MS/MS for the pharmacokinetic study of antituberculosis drugs in blood

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Palavras Chave:*tuberculosis,liquid chromatography,medicine,analytical method,blood plasma*

Highlights

Development of an analytical methodology with liquid chromatography capable of detecting antituberculosis drugs in blood plasma.

Resumo/Abstract

Tuberculosis is a disease that requires global attention, as it is classified as one of the diseases caused by a single infectious agent that kills the most in the world. The drugs used are based on combined fixed dose, also called first-line treatment, which includes the antibiotics isoniazid (INH), rifampicin (RIF), pyrazinamide (PZA) and ethambutol (EMB). A robust LCMS/MS methodology was developed and validated according to Brazilian Health Regulatory Agency (ANVISA) guidelines, first in water solutions, pursued by plasma solutions. The Ethics Committee of Fundação de Medicina Tropical Dr Heitor Vieira Dourado approved this study protocol (CAAE 77489324.2.0000.0005). The calibration standards were purchased from Sigma Aldrich, INH, RIF, PZA, EMB as main antituberculosis and cimetidine as an internal standard, also the reagents Formic Acid (LC-MS grade) and Acetonitrile (HPLC grade). For the calibration curve, were constructed within eleven-point levels. These concentration ranges for the TB drugs were determined based on the medication patients received in the ICU regarding the limitations of the equipment. The equipment used was LCMS/MS 8045, within HPLC column Shim-pack XR-ODS III 2.2µm 150mm x 2.0mm, mobile phases A: Formic Acid 0.1% and B: Acetonitrile : Formic Acid 0.1%. The standards solutions were prepared within Ultrapure water, using a Milli-Q® purification system. The calibration curve was linear according to results in water and plasma, with R^2>0.99 for all the analytes, on the other hand, isoniazid could be detected in plasma. All the results are at table 1, comparing water samples versus plasma samples. This method has been shown to be selective, precise, accurate, linear for both matrixes, however in plasma samples wasn't possible to detect INH, letting us running new more tests to solve this problem in the future.

Parameter/Analyte	EMB	PIR	RIF	Cimetidine
R^2 (water)	0.9926	0.9961	0.9974	0.9982
R^2 (plasma)	0.9972	0.9963	0.9932	0.9996
F	1,2038	5.8507	0.3767	0.0697
P(F<=f) uni-caudal	0,3840	0.00498	0,0697	0.00012
F crítico uni-caudal	3,0716	2,9782	0,3357	0,3357
LQcalc (µg L^{-1})	10.55	6.15	5.00	4.17

Table 1 - Water and Plasma Validation Parameters

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Vanilla Accord in Perfumes: GC–MS Profiling and Data-Driven Comparison Across Fragrance Groups

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Palavras Chave:*Perfumery,Vanilla accord,GC–MS,Chemical profiling,Chemometrics*

Highlights

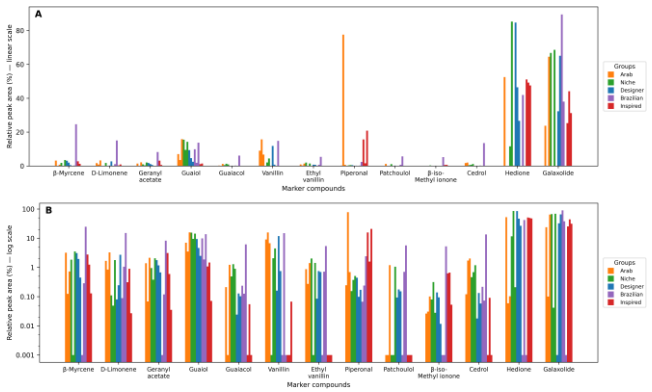
GC–MS feature-based analysis supports profiling of vanilla-related compounds.

Vanilla is not defined by a single molecular marker.

Chemometric workflows enable discrimination among fragrance samples.

Resumo/Abstract

Vanilla accords in perfumes are chemically diverse and cannot be defined by a single molecular marker. This study applied a non-targeted GC–MS workflow to compare 15 commercially available perfumes distributed into five groups (Arab, Niche, Designer, Brazilian, and Inspired; n = 3/group) to evaluate analytical differences in vanilla-related chemical signatures. Fragrance concentrates were diluted 100× in dichloromethane and analyzed on an Agilent 7890A/5975C system equipped with an HP-5MS column (30 m × 0.25 mm × 0.25 µm) using pulsed split injection and full-scan acquisition (m/z 50–500). Data processing in MZmine 2.53 (ADAP chromatogram building, wavelet deconvolution, alignment and gap filling) generated 749 aligned features. Arab perfumes showed the highest mean relative contributions of vanillin-like, ethylvanillin-like and 137/138 vanillic fragments (4.071%, 0.103% and 1.730%), followed by Niche (2.568%, 0.131%, 1.236%), Designer (2.309%, 0.078%, 0.444%), Brazilian (1.366%, 0.056%, 0.743%) and Inspired fragrances (0.013%, 0.000%, 0.023%). Chromatographic complexity also varied among groups, with Niche samples generally presenting fewer detected features per chromatogram and cleaner peak profiles than Inspired fragrances. The highest vanillin-like relative areas were observed in AR7 Liquid Brun (5.005%), AR5 Rifaqaat (4.136%) and NCH9 PDM Althair (4.095%), while ethylvanillin-like signals were highest in NCH1 Grand Soir (0.272%). Exploratory chemometric analysis indicated higher intragroup cohesion for Inspired samples (cosine similarity = 0.776), followed by Brazilian (0.679), Designer (0.671), Niche (0.501) and Arab fragrances (0.474). Compound annotation corresponds to Level 3 identification based on EI spectral matching against NIST libraries, and retention index confirmation is ongoing. These results demonstrate that vanilla accords arise from multiple chemical signatures rather than a single marker.



GC–MS feature-based profiling of marker compounds: (A) proportional scale; (B) log scale.

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BEA - Alimentos e Bebidas

Aroma-driven volatilome of green Amazonian Robusta coffee for future food and cosmetic applications

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Palavras Chave:*Coffea canephora,Untargeted metabolomics,HS-SPME/GC-MS,Chemometrics,Overall quality*

Highlights

Amazonian coffees showed distinct aromatic profiles depending on their origin;

A total of 71 volatiles were annotated;

Indigenous coffee stood out for its higher diversity of volatiles.

Resumo/Abstract

Coffea canephora L. Pierre ex A. Froehner (var. robusta) accounts for approximately 44% of global coffee production. In the Brazilian Amazon region, its cultivation has expanded mainly across the states of Rondônia, Amazonas, and Acre. The aroma of green coffee represents a promising opportunity for applications in the food and cosmetic industries, which have increasingly developed green coffee–based products. However, the aromatic profile of high-quality C. canephora remains largely unexplored. To address this gap, an aroma-driven study was conducted to characterize 50 green coffee samples from Amazonas, Rondônia (including the Indigenous Lands of Sete de Setembro and Rio Branco), and Acre using headspace solid-phase microextraction associated with gas chromatography coupled to mass spectrometry (HS-SPME/GC–MS) in an untargeted metabolomics approach, followed by multivariate analysis. Coffees from Amazonas exhibited the highest total peak areas for alcohols, carboxylic acids, and terpenes. Samples from the Sete de Setembro Indigenous Lands showed the highest total peak areas for esters, ethers, and caffeine. Coffees from the Rio Branco Indigenous Lands exhibited the highest total peak area for alkanes. Samples from Acre showed the highest total peak areas for aldehydes, ketones, and furans. These compounds contribute to desirable sensory attributes, including fruity, herbal, floral, spicy, caramelized, and chocolate-like notes. The multivariate analysis showed that coffee origin strongly influences their aromatic profile and is also associated with their predetermined overall quality. Samples from Sete de Setembro indigenous were clearly differentiated from those from Acre, while samples from Rio Branco indigenous and Amazonas were distributed between these two groups. Overall quality had a marked impact, with samples scoring close to 90 sensory points exhibiting an opposite behavior compared to samples scoring below 80 points.

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Assessment of coffee infusions quality from street commerce in Salvador-BA: an evaluation of microplastic content and elemental composition.

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Palavras Chave:*Microplastic,Coffee infusion,Polypropylene,Street-sold,Beverage*

Highlights

Microplastics (MP) and Ca, Cu, Fe, K, Mg, Mn and P were quantified in street-sold coffee infusions served in glass and PP cups

MP levels (24–67 MP/150mL) showed no significant difference between groups

Resumo/Abstract

Coffee infusions are traditionally street-sold beverages, part of the street-trading culture of Salvador, Bahia[1]. Due to the ubiquitous presence of microplastics (MP)[2], coffee infusion may contain MP derived from food containers and from environmental contamination[3]. Nonetheless, these MPs can act as carriers of other contaminants and adsorb inorganic species due to their surface characteristics[4]. Thus, this work aims to quantify the MP and mineral content of coffee infusions served in polypropylene (PP) from street commerce in Salvador, Bahia. The sampling occurred in three different locations (Ondina (O), Garibaldi (G) and Canela (VC)) in 2 different days, then the coffee infusion collected were divided into two groups: control group (C), (n=3, served in glass cups) and plastic group (A), (n=3, served in PP cups) all filled up with 150 mL of samples. The C and A samples were subjected to alkaline digestion (10% w v^{-1} KOH and 2% v v^{-1} H_2O_2) to quantify MP particles by stereomicroscopy (Stemi 305, Zeiss). For ICP OES analysis, the groups were acid-digested (3.57 mol L^{-1} HNO_3 and 30% w w^{-1} H_2O_2) in a digester block system (180 ºC, 2 hours). The MP content in the coffee infusions analyzed ranged from 24±6 to 67±11 MP/150 mL, no significant difference ($p > 0.05$) was observed between groups C and A. The content of Ca, Cu, Fe, K, Mg, Mn, and P present in coffee infusion samples was determined (Table 1). For all samples, there was no significant difference ($p > 0.05$) in analyte content between groups A and C. However, showed a 19±4% decrease in the one group A sample compared to the C sample at the same location, with a significant difference in Fe content ($p = 0.0008$). Possible interaction between MP derived from polypropylene cups and Fe content in coffee infusions will be investigated in further investigations.

Samples (day)	Ca		Cu		Fe		K		Mg		Mn		P	
	C	A	C	A	C	A	C	A	C	A	C	A	C	A
O (1)	36±2	33.7±0.2	0.17±0.01	0.163±0.005	0.36±0.01	0.291±0.005	1102±41	1141±6	86±3	89.7±0.8	0.25±0.01	0.259±0.003	134±9	141±5
O (2)	33.9±0.6	34.4±0.3	0.210±0.001	0.2109±0.0005	0.30±0.02	0.282±0.003	1109±15	1122±5	86±1	87±1	0.194±0.005	0.20±0.01	134±3	138.1±0.5
G (1)	27±4	26.0±0.6	0.21±0.01	0.206±0.001	0.42±0.04	0.33±0.01	799±115	791±21	56±8	54±1	0.072±0.004	0.068±0.004	68.8±0.6	74±2
G (2)	26±4	23±2	0.21±0.02	0.22±0.02	0.31±0.04	0.26±0.02	642±96	592±49	55±9	52±4	0.063±0.004	0.084±0.002	79±14	98±8
VC (1)	25±1	25±2	0.189±0.002	0.20±0.01	0.28±0.01	0.28±0.03	730±27	729±36	65±3	64±3	0.11±0.01	0.11±0.01	99±5	99±5
VC (2)	25±3	23.9±0.6	0.206±0.002	0.206±0.001	0.27±0.01	0.252±0.003	656±72	612±14	60±7	57±1	0.097±0.002	0.097±0.005	96±11	90±4

Elemental content of coffee infusions (mg/L) served in PP cups (A, n=3) and glass cups (C, n=3).

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Authentication of Whey Protein Using Miniaturized NIR and One-Class Modeling

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Palavras Chave:*Whey Protein,classification,DD-SIMCA,OC-PLS,NIR spectroscopy.*

Highlights

Combining NIR and OCC captures intraclass variability, enhancing detection of adulterated simples; One-Class Classification enables detection of subtle adulterations in whey protein;

Resumo/Abstract

Whey protein (WP) is a widely consumed dietary supplement regulated by agencies such as the FDA and EFSA and used to improve physical performance. Its popularity, complex composition, and lack of standardized regulations make WP products susceptible to adulteration, compromising their biological efficacy. Detecting adulterants is challenging due to the variety of substances added. In this context, near-infrared (NIR) spectroscopy is a fast, non-destructive, and effective alternative, especially when combined with one-class classification (OCC) models such as Data-Driven SIMCA (DD-SIMCA) and One-Class Partial Least Squares (OC-PLS), which model only authentic samples and detect subtle adulteration without requiring information on adulterated classes [1]. In this study, 59 pure whey protein concentrate (WPC) samples and 66 adulterated samples with soy extract (0.1–10%), milk, starch, and wheat (10–40%), including mixtures, were analyzed using MicroNIR™ 1700 and FT-NIR Frontier with diffuse reflectance. Spectra were preprocessed using SNV and MSC, and the sample sets were divided using the Kennard–Stone algorithm[2]. Both DD-SIMCA and OC-PLS models showed satisfactory performance for both instruments. Increasing the confidence level from α = 0.05 to α = 0.01 corrected misclassifications in Frontier without affecting MicroNIR. The McNemar test[3] indicated no significant differences between models or instruments, MicroNIR (p = 1.00) and Frontier (p = 0.48); at α = 0.01, no discordances were observed in the test sets. In conclusion, miniaturized near-infrared spectroscopy combined with OCC provides a rapid, reliable, and non-destructive approach for food authentication, demonstrating efficiency in detecting adulteration in whey protein products.

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Avaliação analítica de suplementos proteicos à base de soro do leite: determinação de proteínas, amido e conformidade da rotulagem

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Palavras Chave:*Controle de qualidade,Suplementação alimentar,Metodologias analíticas*

Highlights

Protein content in whey-based supplements was quantified using validated analytical methods. Experimental results were compared with nutritional values declared on product labels

Resumo/Abstract

O consumo de suplementos nutricionais, especialmente aqueles à base de proteína do soro do leite (*whey protein*), tem apresentado crescimento expressivo, impulsionado por aplicações no esporte e na indústria de alimentos, tornando essencial a avaliação analítica da conformidade entre a composição real e as informações declaradas nos rótulos. Este estudo teve como objetivo determinar o teor de proteínas e investigar a presença de amido em suplementos proteicos comercializados em Imperatriz–Maranhão-Brasil, comparando os resultados experimentais com os valores informados pelos fabricantes por meio de tratamento estatístico. Foram analisadas nove amostras, preparadas segundo metodologias padronizadas. A determinação do teor proteico foi realizada por espectrofotometria UV/Vis a 540 nm, empregando o método do Biureto, enquanto a detecção qualitativa de amido foi conduzida com solução de Lugol. A curva analítica apresentou excelente linearidade, evidenciando a adequação do método analítico. Os resultados indicaram que aproximadamente 89% das amostras apresentaram teores de proteína inferiores aos declarados nos rótulos, com erros relativos superiores a −20%, configurando não conformidade com a legislação brasileira vigente. Tais diverenças foram confirmadas, estatisticamente, com aplicação do teste t de*Student*. A metodologia do Biureto foi validada por comparação com o método de referência de Kjeldahl, não sendo observadas diferenças estatisticamente significativas entre os métodos ($p > 0,05$), o que comprova a exatidão, a reprodutibilidade e a confiabilidade do procedimento analítico empregado. Ademais, cerca de 56% das amostras apresentaram presença de amido não declarado, indicando possível alteração de natureza econômica e comprometimento da qualidade nutricional. Os resultados evidenciam a relevância do monitoramento da qualidade de suplementos alimentares, contribuindo para o controle, fiscalização regulatória e a segurança alimentar e nutricional.

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Breast milk vs. infant formula: nutritional contribution of inorganic elements for full-term neonates

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Palavras Chave:*Bioavailability, Caco-2 cells, Colostrum, Digestion models, Food safety*

Highlights

An infant-specific in vitro digestion model was applied for colostrum. Colostrum shows higher micronutrient bioaccessibility than infant formulas despite lower levels.

Resumo/Abstract

Breastfeeding is essential for the physiological development and maturation of infants during the first days of life. However, despite WHO recommendations, only about 44% of infants under six months are exclusively breastfed, while a portion receive infant formula either partially or exclusively. The reasons include breastfeeding difficulties, nutritional needs, and socioeconomic factors. Differences in the bioavailability of inorganic elements between human milk and formulas may compromise adequate nutritional intake, contributing to nutritional imbalances and potential long-term health consequences. In this context, the present study aimed to evaluate the*in vitro*bioavailability of inorganic elements in colostrum from mothers assisted at the Human and Maternal-Infant Milk Bank (CEP number 5.496.177) and in commercial formulas intended for full-term infants up to 28 days old. The assessment was conducted using a gastrointestinal digestion protocol specifically designed for this age group (Ménard, O.*et al.*, 2018) and*in vitro*bioavailability assays. In human colostrum, the results revealed minor concentrations of Cu, Fe, and Zn (0.5–6.0 mg L^{-1}), as well as Mg (25–45 mg L^{-1}). In infant formulas, Cu and Fe were present at relatively high levels (5.0–8.0 mg L^{-1}), while Mn and Zn occurred at lower levels. Higher bioavailability of Cu and Zn was observed in colostrum (31% and 24% w/w) compared to infant formulas (12% and 7.5% w/w). Ongoing analyses are evaluating the bioaccessibility of Ca and P. To further understand and correlate these findings,*in vitro*bioavailability studies using Caco-2 cells are being conducted, enabling the assessment of the nutritive and/or toxic potential of inorganic elements present in colostrum and formulas, as well as their effects on infant health.

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Bridging Science and Society: Technological and Extension Approaches to PANCs as Sustainable Food Colorants

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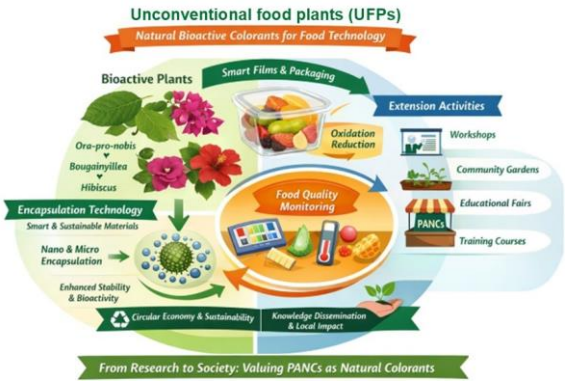
Palavras Chave:*Unconventional food plants (UFPs),Bioactive colorants,Encapsulation technology,Smart packaging,Extension activities*

Highlights

Unconventional food plants as sustainable food sources.
PANC pigments as natural food colorants.
Nanoencapsulation improves pigment stability.
Smart materials with bioactive plant dyes.

Resumo/Abstract

Unconventional food plants (UFPs) are interesting sources of bioactive compounds that contribute to dietary diversification, nutritional security, and the valorization of biodiversity. UFPs contain natural pigments, such as anthocyanins, with great potential for application as natural colorants, meeting the growing demand for healthier and more sustainable food products. This study aims to evaluate the potential of Hibiscus, Pereskia aculeata, and Bougainvillea as sources of natural pigments and its encapsulation to enhance its bioactivity and to promote stability of food products. The methodology involved aqueous/ethanolic (50%) extraction of bioactive pigments from selected UFPs, followed by encapsulation with alginate matrix. The encapsulated materials were subsequently incorporated into functional films to form a smart edible packaging for apple slices. Stability spectrophotometric analyses were conducted to evaluate their effects on oxidative processes and food preservation using DPPH and TBARs assays. In parallel, extension activities (fairs and community initiatives) were used to spread the meaning about UFPs and their sustainable and technological uses.The results demonstrated that encapsulation significantly improved the stability of color and bioactive properties under environmental stress conditions. The incorporation of encapsulated pigments into smart films showed promising results in reducing oxidative degradation in minimally processed fruits and enabling potential applications in food quality monitoring. In addition, extension initiatives contributed to increasing public awareness of UFPs, promoting sustainable resource use, and encouraging the recovery of traditional knowledge and local income generation. Overall, the integration of research, innovation, and extension activities highlights the potential of UFPs as sustainable sources of natural and functional ingredients for the development of advanced and innovative materials for the food industry.



Research-driven schematic illustration showing the valorization of UFPs.

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Can bioactive compounds and smartphone-based analysis be used to classify cocoa content from chocolate?

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Palavras Chave:*Proanthocyanidins,Quality control,Colorimetric analysis,RGB,Multivariate analysis*

Highlights

Proanthocyanidin contents determined by smartphone-based colorimetry discriminate cocoa content; Random Forest achieved 93.9% accuracy (κ = 0.92); Image-based flavan-3-ol data outperformed NIR spectra.

Resumo/Abstract

The characterization of cocoa content in chocolate products is essential for quality control and adulteration detection. Cocoa processing affects bioactive compounds, particularly flavan-3-ols, influencing nutritional properties. Near-infrared spectroscopy (NIR) is a rapid and non-destructive approach, but cost and instrumental requirements limit its use in low-resource settings. This study proposes a low-cost alternative exploring smartphone-based digital image determination of flavan-3-ol markers (total proanthocyanidins and procyanidin B2) and chemometric/machine-learning tools to classify chocolates by cocoa content. Assays used 10 mg of cryogenically ground samples in 1.5 mL microtubes. Total proanthocyanidins were determined by acid hydrolysis (80% v/v ethanol, 1 mol L^{-1} HCl, 60 °C, 60 min), while procyanidin B2 was quantified using the dimethylaminocinnamaldehyde reaction. Images were acquired under controlled illumination with a smartphone camera (Samsung S25 Ultra, 200 MP, f/1.7) and converted to RGB, CMY, and CIELab color systems using ColorGrab®. Images of the ground samples were also evaluated. Unsupervised analysis (HCA and PCA) of 33 samples (0–100% cocoa, 27 variables, 891 data points) showed groupings consistent with labels, separating white chocolates, samples with unknown cocoa content, and high-cocoa levels. Random Forest (RF) with 5-fold cross-validation was highly effective (93.9% accuracy, κ = 0.92, AUC = 0.997); misclassifications occurred only at 30–45% cocoa, while 89% of unknown-content samples were correctly classified. RF importance indicated G, L*, a* and M (proanthocyanidins), R and a* (procyanidin B2), and a* and b* (ground images) as predictors. For comparison, NIR spectra (SNV + derivative) analyzed by RF performed worse (84.9% accuracy, κ = 0.81, AUC = 0.934). Overall, smartphone imaging with simple flavan-3-ol assays can outperform NIR, offering a green and cost-effective workflow for chocolate screening and quality control.

Agradecimentos/Acknowledgments

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Caracterização bromatológica da folha in natura e da farinha do Quiabeiro (Abelmoschus esculentus (L.) Moench) cultivadas no estado de Sergipe

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Palavras Chave:*Composição centesimal,PANC,quiabeiro*

Highlights

Caracterização físico-química e nutricional (atividade de água, umidade, cinzas, proteínas, lipídios e carboidratos totais) das folhas*in natura*e da farinha do*Abelmoschus esculentus*(L.) Moench.

Resumo/Abstract

As Plantas Alimentícias Não Convencionais (PANC) destacam-se pelo seu potencial nutricional, configurando-se como alternativas promissoras para a diversificação da alimentação humana. O quiabeiro (*Abelmoschus esculentus*(L.) Moench) é amplamente cultivado no Brasil, com consumo tradicionalmente associado aos frutos, enquanto suas folhas permanecem pouco exploradas e consumidas, sendo classificadas como PANC. Nesse contexto, o presente estudo teve como objetivo realizar a caracterização físico-química e nutricional das folhas de quiabeiro*in natura*e da farinha obtida a partir das mesmas, cultivadas no estado de Sergipe. As folhas foram cultivadas sem o uso de agrotóxicos, colhidas após 45 dias e submetidas a processos de higienização e sanitização. Parte do material foi analisada*in natura*e outra parte foi seca em estufa com circulação de ar a 40 °C por 72 horas, seguida de trituração para obtenção da farinha. As análises de atividade de água, umidade, cinzas, proteínas, lipídios e carboidratos totais foram realizadas conforme metodologias da AOAC e IAL, em triplicata. Os resultados demonstraram que as folhas*in natura*apresentaram elevada atividade de água (0,98 Aw) e alto teor de umidade (77,19%), indicando maior suscetibilidade à deterioração. A farinha apresentou redução significativa desses parâmetros (0,48 Aw e 9% de umidade), evidenciando maior estabilidade. Observou-se aumento nos teores de cinzas (13,68%), proteínas (23,43%), lipídios (8,36%) e carboidratos totais (45,53%) na farinha, indicando concentração dos componentes nutricionais após o processo de secagem. Conclui-se que a farinha das folhas de quiabeiro apresenta maior estabilidade físico-química e perfil nutricional mais concentrado em comparação à folha*in natura*, mostrando-se uma alternativa promissora na indústria alimentícia, podendo ser incorporada em produtos de panificação e massas, como substituição das farinhas tradicionais, visando o aproveitamento integral dessa espécie como PANC.

Comparative Analysis of Portable and Benchtop NIR Spectrometers for Methanol Quantification in Distilled Spirits

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Palavras Chave:*NIR, PLS, Methanol, Beverages*

Highlights

Methanol poisoning requires rapid screening of spirits. Methanol identified and quantified with portable/benchtop NIR instruments. Methanol is better assigned by combination NIR spectral region.

Resumo/Abstract

The year 2025 was marked by incidents of methanol poisoning associated with the consumption of distilled alcoholic beverages, resulting in fatalities. These occurrences highlight the importance of food safety and control. Given this, the present study aims to compare near-infrared (NIR) methods developed using benchtop and portable devices to identify and quantify methanol in different types of alcoholic beverages. Thirty-nine commercial samples of alcoholic beverages were used, including 6 Cachaças, 11 Gins, 11 Vodkas, and 11 Whiskeys. The samples were adulterated using two mixture designs. The first design involved a ternary mixture of ethanol, methanol, and water. The second design was based on the use of pseudo components, varying the proportions of distilled beverage, methanol, and ethanol. In both cases, the methanol content ranged from 0% to 16.67% (v/v). These designs were employed to ensure that there was no correlation between the methanol and ethanol content, thus indeed quantifying methanol. Subsequently, the samples were analyzed using a PerkinElmer benchtop spectrometer, as well as MicroNIR and NeoSpectra portable devices. Principal component analysis (PCA) indicated both the NeoSpectra portable and the benchtop NIR spectrometer were able to identify methanol in the samples. The chemical information associated with this analyte is predominantly presented in the region of the combination bands, specifically around 1930 and 2303 nm. Partial least squares (PLS) regression models were developed and compared. The model obtained with spectra recorded in MicroNIR achieved RMSEP of 1.22% (v/v) and R^2 of 0.95, while NeoSpectra proved RMSEP of 0.61% (v/v) and R^2 of 0.99. The best performance was observed for the benchtop NIR spectrometer, with an RMSEP of 0.36% (v/v) and R^2 of 0.99. These results evidenced that NIR spectroscopy using portable and benchtop instruments enables identification and quantification of methanol accurately.

Agradecimentos/Acknowledgments

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Determination of mercury in the CRM candidate of black cricket flour (Gryllus assimilis)

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Palavras Chave:*Certified Reference Material,Insects,mercury,food safety*

Highlights

The use of insects as Certified Reference Material is interesting due to their significant nutritional importance. Quantifying mercury in this matrix is important to verify potentially toxic levels.

Resumo/Abstract

Certified Reference Materials (CRM) play an important role in method validation and quality assurance, being indispensable for the traceability and reliability of analytical results. In this sense, it is essential to have CRM that include different matrices, such as insects of great interest to the food industry. It is estimated that around 2 billion people worldwide consume insects because they are more economically viable compared to conventional sources, due to their low production cost and high feed conversion efficiency. However, in Brazil, there is still no CRM for insects such as the black cricket. Among the elements of interest in a CRM, Hg stands out, which has high toxicity and is an important parameter for food safety in edible insects that are bioaccumulators and can compromise the biological integrity of the consumer. From this perspective, the samples were initially ground and lyophilized, and after microwave-assisted acid digestion, hydroxylamine hydrochloride was added, acting as a reducing agent and eliminating excess HNO3. Next, Hg quantification was performed using Cold Vapor Atomic Absorption Spectrometry (CV-AAS) on the samples of CRM candidate of black cricket flour (Gryllus assimilis), previously prepared in the laboratory. In this method, Hg2+ is reduced to Hg0 in the presence of the reducing agent SnCl2. However, the results obtained with an internal standard of homogeneity known for mercury indicated that the method employed showed low recovery, with an average value of 75.49%, below the value accepted by INMETRO (80-120%). Therefore, an adapted methodology from Akagi and Nishimura (1991) was chosen, using a mixture of HNO3, H2SO4, and HClO4 and a heating plate, which proved to be a promising alternative for Hg quantification. Further studies will be conducted to validate the method.

Agradecimentos/Acknowledgments

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Determination of the mineral composition and nutritional assessment of cassava flour consumed in Salvador, Brazil

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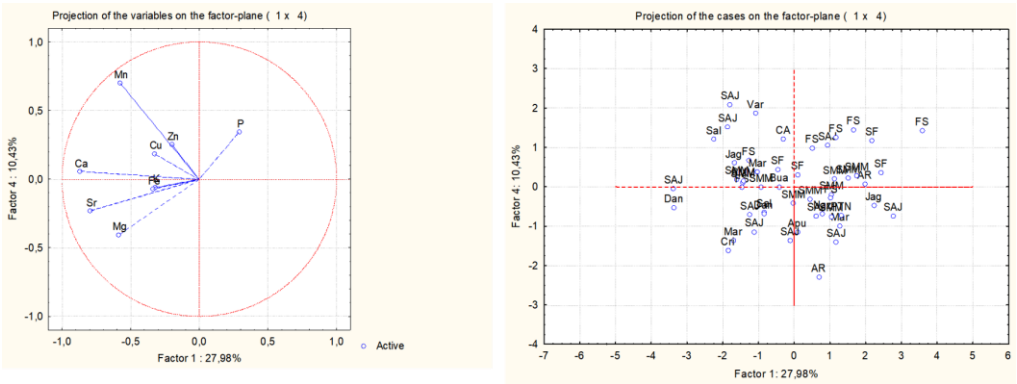
Palavras Chave:*Cassava flour,nutritional assessment,mineral composition,recommended dietary intake,PCA*

Highlights

A nutritional assessment of cassava flour consumed in Salvador was conducted. Fifty samples were purchased from different regions of the city. Manganese and iron are important nutrients in this food.

Resumo/Abstract

Cassava flour, beans, and rice are the main carbohydrate sources in the diet of Salvador, Bahia. This work is conducted as part of a project to determine the nutritional profile and assess the risks associated with potentially toxic chemical elements in cassava flour consumed in this city. Fifty flour samples were purchased, digested in a microwave oven, and analyzed by ICP OES. The average values, expressed in mg of chemical element per 100 grams of flour, were: 303 for K, 65 for Ca, 57 for P, 46 for Mg, 1.7 for Fe, 0.77 for Zn, 0.46 for Mn, and 0.057 for Cu. The nutritional assessment is calculated as the ratio of the nutrient content in a sample to the recommended dietary intake (RDI) of that nutrient. The RDI values are established for each nutrient based on an individual's sex and age. For men aged 19 to 30 years, these values are: 3,400 mg for K, 1,000 mg for Ca, 700 mg for P, 400 mg for Mg, 8 mg for Fe, 11 mg for Zn, 2.3 mg for Mn, and 0.9 mg for Cu. Based on these data, considering a daily intake of 100 g of flour, the percentage contributions of the flour to the daily nutrient intake were estimated as: 21.3% for Fe, 20% for Mn, 11.5% for Mg, 8.9% for K, 8.1% for P, 7.0% for Zn, 6.5% for Ca, and 6.3% for Cu. Based on the estimated contribution percentages of the micronutrients present in cassava flour, it is observed that this food has greater nutritional relevance for Fe and Mn, indicating that its consumption can significantly contribute to the daily intake of these elements, particularly in the context of the need for iron in diets aimed at preventing and controlling iron-deficiency anemia. However, Mg makes a moderate contribution, whereas K, P, Zn, Ca, and Cu have limited contributions. The assessment of nutrient levels in the fifty flour samples was also performed using PCA and HCA. The results did not indicate the formation of clusters; however, the graphs highlight some samples due to their high phosphorus content.



PCA score plot of samples and loading plot showing chemical element contributions.

Agradecimentos/Acknowledgments

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Development of Intelligent Starch-Based Packaging Using Açaí Anthocyanins

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Palavras Chave:*Intelligent packaging,starch,anthocyanins,açaí,biodegradable materials*

Highlights

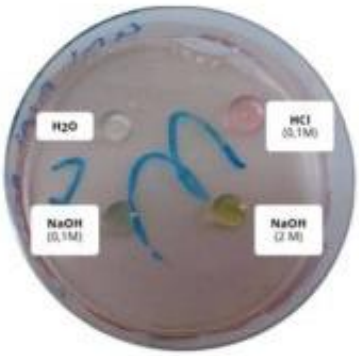
Intelligent biodegradable packaging was developed using starch and açaí

Anthocyanins in açaí change color with variations in pH

Visual color change allows rapid detection of degradation of packed food

Resumo/Abstract

Açaí is a Brazilian fruit rich in anthocyanins, which undergo color changes in response to the pH of the environment. The goal of this work is to develop intelligent, biodegradable packaging materials based on starch films incorporated with açaí extract, aiming detection of food degradation by color change. Anthocyanins present in açaí flour were extracted in an aqueous medium, and the starch-based films were produced by the casting method, using glycerol as a plasticizer. Gelatinization of starch was carried out at 85-90°C, after which, the aqueous açaí extract was incorporated at room temperature to avoid its thermal degradation, under constant mechanical stirring to ensure homogeneous incorporation into the filmogenic solution. The films were dried in a lab oven at 45ºC for ~24 hours. The films obtained were characterized using RGB (Red, Green and Blue) colorimetric analysis, based on photographs taken with a smartphone. In addition, a qualitative spot test analysis demonstrated the difference in a film coloration when adding hydrochloric acid (HCl) or sodium hydroxide (NaOH) solutions, both at a concentration of 0.1M. The original reddish coloration of the films changed to pink under acidic conditions and to green in a basic medium. A higher NaOH concentration (2.0M) resulted in a yellow film. We have also performed experiments using films as packages of meat and chicken. We observed color changes during the food spoilage process. These results demonstrate that the potential of the developed films for rapid and visual monitoring of food degradation through packaging color changes, offering an accessible tool to assist consumers at the point of purchase. Furthermore, this study presents a sustainable technological alternative to conventional petroleum-based plastic films used for packaging, contributing to the development of environmentally friendly biodegradable materials.



Film color response: HCl 0.1M (pink), NaOH 0.1M (green), NaOH 2.0 M (yellow), water (transparent).

Agradecimentos/Acknowledgments

The authors thank FAPESP (grant no. 2025/25043-1 and 2025/09383-7), CAPES, and CNPq for the financial support provided for the development of this work.

Discrimination of Jataí stingless bee honey by FTIR-ATR as a non-target method

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Palavras Chave:*meliponiculture, geographic location, chemical profile, chemometrics.*

Highlights

FTIR was used as a non-target tool for Jataí stingless bee honey.

Samples could be differentiated by PCA, mainly due to the influence of plants used as shepherding for bees.

Resumo/Abstract

Meliponiculture is an important productive activity, and due to the diversity of native bee species, the location of the hives, the type of flowering, and the time of year, honeys with different aromas and flavors have emerged, highlighting the importance of differentiating between these honeys and their origin. This study addresses the influence of different regions on the profile of honeys produced by the Jataí bee (*Tetragonisca angustula*), using FTIR-ATR as a non-target methodology, using Principal Component Analysis (PCA) using the entire spectrum as input variables, and the Origin2024® software. Samples were collected directly from the pots in the hives using a hypothermic plastic syringe and stored in closed Falcon tubes from eight different producers distributed between the rural and urban areas of the municipality of Toledo, Paraná, Brazil. The samples were evaluated using a PerkinElmer Frontier® FTIR scanner with an Attenuated Total Reflectance (ATR) module, in the range of 4000 to 600 cm^{-1}, with a resolution of 2 cm^{-1} and 16 scans. Figure 1 presents the PCA graph showing the differentiation between the samples, with PC1 and PC2 explaining 99.12% of the data. The samples from producers 7 and 8 differ in PC1 (95.70%) from the others, both being in urban areas, as are producers 1, 2, 4, and 6. Producers 3 and 5 are in rural areas, indicating that this is not the discriminating factor. The difference observed in samples 7 and 8 can be explained by the fact that, exclusively in these locations, producers cultivate the*Antigonon leptopus*plant near the beehives. This plant has continuous and abundant flowering throughout the year, and its flowers contain substances such as saponins, tannins, coumarins, glycosides, terpenes, and flavonoids, among others, which influence the characteristics of the honey produced.

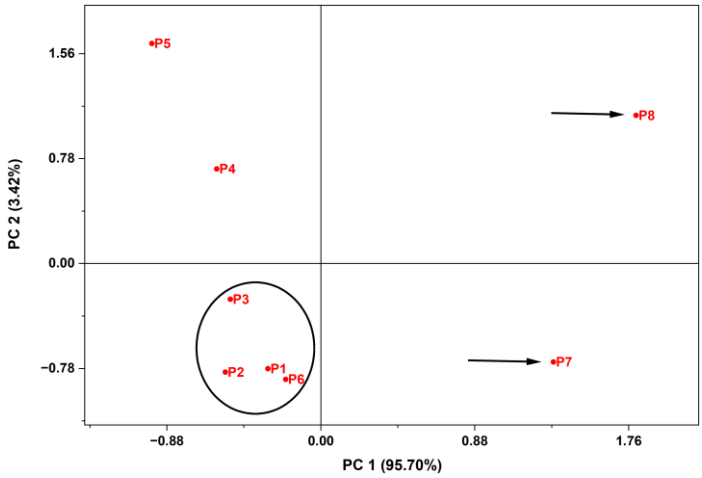


Fig 1. Score plot (PCA) for honey samples from FTIR variables.

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Elemental Fingerprinting and Chemometric Tools for the Authentication of Brazilian Geographical Indication Coffees Using Portable X-Ray Fluorescence

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Palavras Chave:*Multielemental Profiling,pXRF,GI,Classification*

Highlights

pXRF enabled rapid and non-destructive multielemental analysis of Brazilian GI coffees. PCA revealed natural clustering and regional discrimination based on elemental profiles.

Resumo/Abstract

Geographical indications (GIs) for Brazilian coffees certify the relationship between origin and quality, playing a strategic role in adding value to these products. However, the high added value of these products increases their vulnerability to fraud, thus requiring robust, rapid, and practical analytical methodologies for origin authentication. This study investigates the application of portable X-ray fluorescence spectrometry (pXRF), combined with chemometric tools, for the authentication of coffees from four Brazilian regions. A total of 20 samples from each selected region were analyzed: Mata de Minas, Cerrado Mineiro, Mantiqueira de Minas, and Mogiana. The pXRF technique enables direct multielemental analysis without sample preparation, making it a practical, non-destructive alternative. The obtained data were subjected to Principal Component Analysis (PCA), which revealed a clustering tendency and natural separation among the regions, mainly observed along principal components PC1 and PC2, explaining 53.44% of the total variance. These results indicate that the elemental profile exhibits discriminant potential. Further investigations employing supervised classification models, such as SIMCA and DD-SIMCA, will be conducted to validate the statistical robustness of the proposed authentication models.

Agradecimentos/Acknowledgments

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Enriquecimento de esfiha aberta com farinha da folha de abóbora (Cucurbita moschata D): perfil físico-químico e nutricional

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Palavras Chave:*PANC;Folha;Abóbora;Esfiha;Farinha*

Highlights

Massa de*esfiha*aberta enriquecida com farinha de folha de abóbora (PANC). A formulação F2 aumentou proteínas, lipídios e vitamina C e reduziu carboidratos em comparação com o controle.

Resumo/Abstract

As Plantas Alimentícias Não Convencionais (PANC) que são espécies e partes comestíveis ainda subutilizadas, constituem um recurso relevante para diversificar a dieta e melhorar a qualidade nutricional das refeições. Sua utilização pode contribuir para a redução de custos e para o fortalecimento da segurança alimentar, especialmente em contextos de disponibilidade local. Do ponto de vista ambiental, também incentivam sistemas alimentares mais sustentáveis, com melhor aproveitamento de recursos e menor geração de resíduos. Este trabalho teve como objetivo desenvolver massa de*esfiha*aberta com a incorporação de diferentes concentrações de farinha da folha de abóbora (*Cucurbita moschata*D.): um controle (sem adição) e duas formulações (14,5 g- F1 e 21,5 g- F2 de farinha incorporada em cada). As amostras foram preparadas em condições padronizadas e avaliadas por análises físico-químicas (pH, acidez, umidade) e nutricional (proteínas, lipídios, cinzas, carboidratos e vitamina C). Entre os resultados, verificou-se melhora do perfil nutricional nas formulações enriquecidas quando comparadas ao controle, pois foi observado uma tendência ao aumento progressivo de nutrientes conforme aumentava a concentração de farinha adicionada. A formulação F2 apresentou maiores valores, destacando-se os teores de proteínas (10,37%), lipídios (5,80%) e vitamina C (0,268 mg/100g) e redução do teor de carboidratos (54,02%). Portanto, a incorporação da farinha da folha de abóbora nas*esfihas*demonstrou ser eficaz para aumentar o teor nutricional e agregar valor ao produto final, contribuindo para uma alimentação mais nutritiva e incentivando o aproveitamento de uma matéria-prima vegetal frequentemente descartada por falta de conhecimento.

Agradecimentos/Acknowledgments

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Evaluation of total contents and in vitro bioaccessibility of essential elements in Vernonia polyanthes Less.

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Palavras Chave:*Unconventional food plants (UFPs); In vitro gastrointestinal digestion; Atomic spectrometry; Matrix processing; Food biodiversity.*

Highlights

FAAS used to determine total and bioaccessible mineral contents.

In vitro digestion showed differences between total and bioaccessible fractions.

Processing affected mineral bioaccessibility.

Resumo/Abstract

Unconventional food plants (UFPs) have attracted increasing interest due to their nutritional potential and contribution to biodiversity valorization; however, information on the bioaccessibility of essential mineral elements in these matrices remains limited. In this context, this study aimed to evaluate the total contents and*in vitro*bioaccessibility of essential elements in*Vernonia polyanthes*Less. (assa-peixe), contributing to the analytical characterization of this species with potential food applications.

Samples were subjected to microwave-assisted mineralization for the determination of total element contents and to an*in vitro*gastrointestinal digestion procedure to estimate bioaccessibility. The determinations of Fe, K, Mn, Na, and Zn were performed by flame atomic absorption spectrometry (F AAS). Different sample processing forms were evaluated (fresh, cooked, and extract).

Total contents ranged from approximately 3 to 20 mg/100 g for Fe, 380 to 3900 mg/100 g for K, 0.2 to 2.5 mg/100 g for Mn, 0.5 to 2.3 mg/100 g for Na, and 0.13 to 1 mg/100 g for Zn, depending on plant processing, with the fresh form generally associated with the highest concentrations. Bioaccessibility percentages corresponded to 0.11–1.7% (Fe), 0.02–28% (K), 0.38–41% (Mn), 6.5–33% (Na), and 1.6–10% (Zn), with higher proportional release observed for the extract, demonstrating that total content does not necessarily represent the fraction potentially available for absorption.

The results highlight the importance of analytical approaches that consider nutrient bioaccessibility in addition to total content and contribute to the valorization of*V. polyanthes*as a UFP with nutritional potential, aligned with strategies for food security and sustainable use of biodiversity.

Agradecimentos/Acknowledgments

The authors thank the Federal University of Ouro Preto for institutional support and laboratory facilities. Financial support from FAPEMIG (APQ-00406-21) is also gratefully acknowledged.

Immobilized L-asparaginase for acrylamide mitigation in French fries processing

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Palavras Chave:*L-asparaginase;,enzyme immobilization;,food safety;,acrylamide mitigation;,potato products*

Highlights

L-asparaginase immobilized on SBA-15 for acrylamide mitigation.
L-asparagine as an adjuvant greatly improved activity yield.
Effective L-asparagine hydrolysis in simulated potato blanching experiment.

Resumo/Abstract

The presence of acrylamide in certain aliments raises food safety concerns due to its neurotoxic and genotoxic effects, as well as its carcinogenic potential. Acrylamide is formed during the Maillard reaction between reducing sugars and L-asparagine when foods, such as French fries, bakery products and roasted coffee, are heated above 120 °C. L-asparaginase is a promising enzyme capable of hydrolysing L-asparagine prior to heating, thereby reducing acrylamide formation. In this study, a recombinant Escherichia coli L-asparaginase-based biocatalyst was developed through covalent immobilization onto mesoporous silica SBA-15. Immobilization was performed under three conditions: without additives (SBA-E), with L-asparagine (SBA-E(Asn)), or with L-glutamine (SBA-E(Gln)) as adjuvants. SBA-E(Asn) showed the highest global activity yield (93.4%), followed by SBA-E(Gln) (38.9%) and SBA-E (7.3%). SBA-E(Asn) was further coated with polyethyleneimine, generating SBA-E-PEI, which retained 74.8% of the activity of SBA-E(Asn). Kinetic parameters of the free enzyme and immobilized biocatalysts were evaluated, and SBA-E(Asn) and SBA-E-PEI exhibited higher substrate affinity, with Michaelis-Menten constants of 299 and 314 µM, respectively, compared with the free enzyme (1.773 mM). Operational stability assays demonstrated that both biocatalysts retained over 50% of their initial activity after 10 reuse cycles with L-asparagine at 55 °C, an industrially relevant temperature, with no statistically significant differences between them. Finally, SBA-E(Asn) was applied in a simulated potato blanching process, effectively hydrolysing L-asparagine, as confirmed by increased ammonia release relative to control samples. These results indicate that SBA-E(Asn) is a promising tool for acrylamide mitigation in French fries. Technology derivatives can be applied to coffee and bakery products, although further improvements in stability and formulation are required for industrial application.

Inteligência Artificial e Quimiometria na Garantia da Integridade Alimentar: Estudos de Caso e estratégias para modelagem em campo

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Palavras Chave:*Quimiometria, Inteligência Artificial, Integridade Alimentar, Análise em Campo, Software Livre,Quimiometria,Inteligência Artificial,Integridade Alimentar,Análise em Campo,modelagem em nuvem*

Highlights

- AI and Chemometrics for on-site food integrity.
- Fast, sustainable, and non-destructive field analysis.
- User-friendly GUI solutions developed by LTAP/UERJ.
- Lab-to-farm technology.

Resumo/Abstract

A garantia da integridade alimentar enfrenta desafios crescentes que demandam respostas rápidas e precisas, muitas vezes inviáveis pelos métodos laboratoriais convencionais de alto custo e tempo de resposta elevado. Este trabalho apresenta a integração entre Inteligência Artificial (IA) e Quimiometria como uma estratégia disruptiva para o monitoramento de alimentos diretamente no campo. Discutem-se as vantagens das metodologias analíticas limpas, que eliminam o preparo complexo de amostras e o uso de reagentes tóxicos, utilizando técnicas como espectroscopia NIR e imagens digitais. Apresentamos estudos de caso práticos, incluindo a detecção de fraudes em carnes e adulterações em farinhas de banana, onde modelos de Machine Learning (como XGBoost e SHAP) permitem não apenas a classificação, mas a compreensão dos marcadores químicos relevantes. Por fim, o trabalho destaca o desenvolvimento de interfaces gráficas (GUIs) e web apps (CWA) pelo Laboratório de Tecnologia Analítica e Processos (LTAP/UERJ). Essas ferramentas democratizam o acesso à modelagem quimiométrica robusta, permitindo que análises complexas sejam realizadas em dispositivos móveis e laboratórios itinerantes, como o projeto "Serra Móvel", conectando a ciência de ponta às necessidades reais da produção de alimentos.

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Multiproduct chromatographic analysis of biogenic amines in ten different food matrices.

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Palavras Chave:*Biogenic amines, Multiproduct analysis, Chromatography, Food safety, Quality control.*

Highlights

Single HPLC method quantifies eight biogenic amines in various food via pre-column dansylation and C18 gradient.Validation with good linearity(r>0.98)and recovery tests ongoing for lab implementation.

Resumo/Abstract

Biogenic amines (BAs) are organic bases formed by amino acid decarboxylation during microbial spoilage, where consumption at levels higher than 50 mgL^{-1} (depends on the food) is associated with toxicological effects. BAs are also used as a freshness biomarker in foods. Therefore, their monitoring requires sensitive analytical methods to ensure consumer safety and evaluate product shelf life. A challenge in BA analysis is matrix complexity due to the variety of interferences. Methods validated for only a few specific matrices are commonly found, requiring multiple protocols, which increases costs and complexity. This work aims to develop a chromatographic method for simultaneous analysis of eight BAs (tryptamine, phenethylamine, putrescine, cadaverine, histamine, tyramine, spermidine and spermine) in multiple matrices. Pre-column derivatization is performed to enhance the structure of BAs before chromatographic separation, thereby increasing analyte retention and making them feasible to ultraviolet detection. The separation was carried out using High-Performance Liquid Chromatography, with separation conducted on a C18(2) column (Phenomenex Luna, 150 × 4.6 mm, 100 Å) with temperature controlled at 35°C. The binary elution consists of solvent A: water (18,2MΩ) and Solvent B: acetonitrile and the flow rate was controlled at 1.0 $mL \cdot min^{-1}$. The used gradient provided good resolution of target analytes within a time compatible with routine analyses. Preliminary data, represented by calibration curves, confirmed method feasibility with adequate linearity with $r > 0.98$, homogeneous and no correlated residue. The current stage involves conducting recovery tests in different matrices to evaluate the accuracy and presence of interferents, reproducibility and evaluation of robustness and other validation parameters such as limits of quantification and precision. Interferences will be solved with the second order advantage of the chromatographic data using chemometrics models.

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Multivariate control using z-score data and repeatability standard deviation as metrics in integrated dry matter and ash analyses of feed samples.

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Palavras Chave:*Dry Matter,Ash,Principal Componente Analysis,Partial Least Squares Regression (PLS*

Highlights

Multivariate process control using PCA and PLS with z-score and repeatability SD enabled long-term monitoring of dry matter and ash analyses in Brachiaria, maize and soybean meal, independent of reference material changes.

Resumo/Abstract

The determination of dry matter and ash is fundamental in feed analysis and influences storage, nutritional value and food price. Dry matter corresponds to the fraction remaining after water removal, and ash represents the inorganic residue obtained after combustion of organic matter, reflecting total mineral content. In these gravimetric analyses, process stability depends on multiple operational variables acting simultaneously, which limits the effectiveness of univariate approaches in identifying causes of analytical failures. Multivariate statistical process control has been recognized as a robust tool for integrated monitoring of complex analytical systems. However, the periodic replacement of reference materials from different proficiency testing rounds makes it difficult to maintain traditional control charts over long periods. The objective of this work was to develop a multivariate statistical process control system based on Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS), using results expressed as z-score and repeatability standard deviation for continuous monitoring of the analytical process over time, independent of changes in reference materials. Samples of Brachiaria forage, soybean meal and ground maize were used. Robustness was evaluated using a Youden design with eight experiments and seven operational variables at two levels: air circulation (with or without), sample mass (1 g and 2 g), oven temperature (105 °C and 103 °C), drying time (16 h and 4 h), muffle furnace temperature (600 °C and 550 °C), combustion time (250 and 180 minutes), and air renewal (with and without). More than one hundred analyses under normal operating conditions were used to build the reference model, and sixteen process variations were introduced to evaluate detection capability. The first four principal components explained more than ninety percent of the total variance, and control limits were defined at the 99% percentile of the Hotelling T^2 and Q residual statistics. Results indicate that the use of z-score and repeatability standard deviation enables long-term control charts independent of specific reference materials, allowing continuous monitoring of laboratory metrological performance.

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Multivariate statistical process control for the detection of operational variations in crude fat analysis of animal feed samples

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Palavras Chave:*Controle estatistico multivariado de processos, Extrato Etéreo, Garantia de qualidade analítica,Multivariate Statistical Process Control (MSPC); Crude Fat (Ether Extract); Analytical Quality Assurance.*

Highlights

Multivariate control charts integrating proficiency test reference material data with Principal Component Analysis and Partial Least Squares detect variations in crude fat analysis of feeds.

Resumo/Abstract

The modernization of food testing laboratories requires efficiency, metrological traceability, and quality control. Univariate controls do not always capture simultaneous variations of multiple operational factors, making it difficult to identify the root causes of analytical deviations. In this context, the determination of crude fat (CF) content is essential for energy evaluation and diet formulation in animal feeds. The objective of this work was to develop a multivariate statistical process control (MSPC) system capable of detecting process deviations in the simultaneous determination of dry matter and crude fat. Extractions were performed in an XT10 extractor (Ankom®) using filter bags after drying in an oven at 105 °C. Multivariate control charts of Hotelling T^2 and Q residuals were built from Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS) models. Performance was assessed using z-score measurements and the relative standard deviation of repeatability (RSDr). The analyzed feed matrices were Brachiaria forage, ground corn, and soybean meal from proficiency testing schemes (EPCBO). Official methodologies from MAPA, SINDIRAÇÕES, and IAL were used to define the process variables. Robustness was evaluated using a Youden design with 8 experiments and 7 factors at two levels: sample mass (1.0/0.8 g), extraction temperature (90/100 °C), pre-drying time (4/16 h), extraction time (60/90 min), post-extraction drying time (30/60 min), cooling time (30/60 min), and reusability of filter bags (XT4, Ankom®). PCA and PLS models were calibrated using more than 100 analyses with expected CF behavior, while 16 process variations were introduced for validation through out-of-control events. The system detected variations associated with sample mass and extraction, post-extraction drying, and cooling times, demonstrating potential to anticipate analytical deviations and support root cause identification in routine laboratory operations.

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Multivariate statistical process control of sequential analyses of neutral detergent fiber and acid detergent fiber in brachiaria and soybean meal

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Palavras Chave:*Multivariate Statistical Process Control (MSPC),Crude Fat (Ether Extract),Analytical Quality Assurance.*

Highlights

Statistical Process Control using z-scores and RSDr from dry matter and ash determination of animal feed samples enabled early detection of analytical deviations and improved quality in routine labs.

Resumo/Abstract

Neutral detergent fiber (NDF) and acid detergent fiber (ADF) analyses are widely used in roughages and concentrates to estimate the structural carbohydrate fraction of plants and to predict intake and digestibility, especially in ruminants. NDF represents the fraction composed of hemicellulose, cellulose, and lignin, whereas ADF represents the most difficult-to-digest fraction, composed of cellulose and lignin. Modern determination methods employ the Ankom® extraction system using filter bags. Univariate controls do not always capture simultaneous variations in multiple operational factors, making it difficult to identify the root causes of analytical deviations. To meet analytical quality requirements, Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS) were applied in multivariate statistical process control (MSPC) of data matrices from sequential NDF and ADF analyses performed on brachiaria and soybean meal samples. Soybean meal samples underwent an additional starch removal step using amylase/urea. The Youden robustness design included 8 experiments and 7 critical variables at two levels: sample mass (0.5 g and 0.8 g); filter bag type (Ankom and nonwoven fabric, NWF); NDF extraction time (70 and 75 min); ADF extraction time (60 and 65 min); number of washings (2 and 3); washing time (2 and 15 min); and ADF extraction temperature (95 °C and 100 °C). PCA and PLS models were calibrated using more than 100 analyses with expected behavior for ADF and NDF, while 16 deliberate variations were introduced for validation through out-of-control events. The system detected variations related to sample mass, extraction times (NDF and ADF), and ADF extraction temperature. The multivariate system proved effective in identifying root causes of problems in laboratory fiber analyses.

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Non-carcinogenic risk assessment of essential and potentially toxic elements in Amazonian honeys

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Palavras Chave:*Inorganic elements,honey,ICP-OES,risk indices,Amazon.*

Highlights

Elemental analysis of honey samples from the Amazon region. Health risk was assessed using EDI indices, and HQ and non-carcinogenic HI were calculated for the elements studied.

Resumo/Abstract

In this study, the levels of As, Ba, Ca, Cd, Cr, Cu, Fe, Mg, Mn, and Zn were determined in honey using inductively coupled plasma optical emission spectrometry (ICP-OES). In addition, a risk assessment study was conducted. The honey samples were digested as described by Lemos et al. 2017 [1]. The elements were determined in the samples by ICP-OES. The evaluation of the measurements performed by ICP-OES was assessed using the analyte addition and recovery method. The recoveries obtained ranged from 85.6 to 111.7%. The detection limits (LOD) and quantification limits (LOQ) for As, Ba, Ca, Cd, Cr, Cu, Fe, Mg, Mn, and Zn ranged from 0.002 to 0.40 mg kg^{-1} and 0.01 to 1.32 mg kg^{-1}, respectively. All samples had Ca and Mg contents ranging from 48.5 to 111.4 and 10.6 to 46.1 mg kg-1, respectively. The barium concentrations found in eight samples ranged from 0.6 to 1.2 mg kg^{-1} . As, Cr, Fe, and Mn were below the detection limit in all ten samples studied. Cadmium was detected only in sample A6 (0.03 mg kg^{-1}), while zinc was quantified only in sample A3 (0.4 mg kg^{-1}). Health risk was assessed based on the estimated daily intake (EDI) of Cd, Cu, Fe, and Zn. For all elements, EDI values were below the provisional maximum tolerable daily intake (PMTDI) established by the FAO/WHO JECFA committee [2]. Therefore, all EDI values are in compliance with the tolerable intake. The hazard quotient (HQ) and hazard index (HI) for As, Ba, Cd, Cu, Fe, Mn, and Zn were calculated. The HI values, which consider the sum of the HQs of all elements, ranged from 5.81×10^{-3} to 8.33×10^{-2}, indicating that the overall health risk is low. These values are well below 1, which means that, in general, the samples studied do not pose a significant risk of toxicity and exposure to the elements studied is safe.

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Non-destructive quality control of jatobá fruit using chemometrics models.

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Palavras Chave:*Chemometrics, NIR, Process Analytical Technology, Jatobá, Non-destructive Analysis*

Highlights

Detection of jatobá fruit using near-infrared spectra. Evaluation of supervised models for dataset classification. Potential use to assist in the commercialization of a typically brazilian fruit.

Resumo/Abstract

Jatobá is a fruit native to several Brazilian biomes, known for its versatile flour used in food production. However, assessing its ripeness and freshness via visual inspection is unreliable, complicating commercialization. This study proposes a non-destructive analysis (NDA) approach using chemometrics and supervised classification models to discriminate between spoiled (S) and non-spoiled (NS) fruits without opening them. Specimens were collected from the Cerrado and Atlantic Forest regions, as well as local markets in Rio de Janeiro. A database was built using 346 near-infrared (NIR) spectra acquired from fruit shells using a portable spectrometer (900–1700 nm). Post-analysis, fruits were opened to confirm their status, revealing 66 NS and 280 S samples. Data was partitioned into training (80%) and testing (20%) sets using the Kennard–Stone algorithm. To address the class imbalance, the Synthetic Minority Over-sampling Technique (SMOTE) was applied to the NS training data, resulting in 484 total samples (including 138 synthetic NS samples). Preprocessing involved a first-derivative Savitzky–Golay filter. Six classification models, SIMCA, OCPLS-DA, DD-SIMCA, PLS-DA, SPA-LDA, and GA-LDA, were evaluated. A binary SIMCA model yielded the best performance, achieving 94.23% accuracy on the test set. The analysis was supported by cloud-based web platforms developed by the LTAP research group easily accessed at the link https://www.ltapuerj.com.br/materiais, facilitating real-time data processing and reporting directly at the point of sale. These findings demonstrate that portable NIR spectroscopy, combined with robust classification models, provides an effective, non-destructive method for evaluating jatobá fruit integrity. This preliminary study establishes a foundation for enhanced quality control of jatobá and its derivatives, potentially increasing the market value of this Brazilian resource.

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FAPERJ, CNPq, LTAP, PPGEQ/UERJ, UERJ.

Obtaining carrageenan from the algae Kappaphycus Alvarezii and evaluating its glycemic profile in vivo

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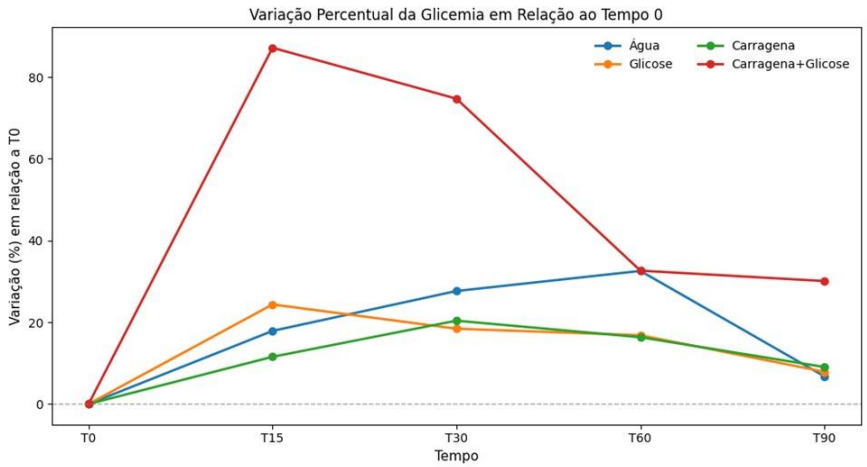
Palavras Chave:*Carrageenan, extract, supplements, Kappaphycus alvarezii.*

Highlights

Development of a sports supplement for athletes based on a biocompound extracted from the algae*Kappaphycus alvarezii*.

Resumo/Abstract

The red algae*Kappaphycus alvarezii*is an important source of biocompounds and nutrients, highlighting carrageenan, a hydrocolloid widely used for its gelling and stabilizing properties, and for its potential medical and bioactive applications in supplements, cosmetics, and treatments. This study aimed to extract carrageenan using two different methods: alkaline hydrolysis and ultrasound. Furthermore, it aimed to evaluate its application in formulating dietary supplements for athletes, aiming for improved physical performance and sustained energy during exercise in a healthy and sustainable way. In the hydrolysis method, the algae underwent alkaline treatment and aqueous extraction. The entire process took approximately 3 days and involved temperature shocks, drying in an oven at 65 °C, and homogenization in a water bath at 80 °C until a uniform gel was obtained, resulting in carrageenan. In the ultrasound extraction method, high-power sound waves were used to break down the algae cell wall, taking approximately 30 minutes to obtain carrageenan with total biomass utilization and using only distilled water. The study also aimed to evaluate, in an animal model, the effects on glycemia of acute and chronic ingestion of the carrageenan gel obtained from the extraction. The process involved separating four groups of 10 mice, each ingesting a different composition: water, carrageenan, glucose, and carrageenan + glucose, for evaluating the glycemic curve at different time intervals. The carrageenan + glucose combination showed a positive synergistic impact on the curve compared to the ingestion of these substances in isolation. Methodological adjustments were made, such as greater control of the extraction, necessary to ensure better purity, stability, and industrial applicability, and to determine the best composition along with carrageenan for improved physical conditioning and minimization of side effects.



Curva da variação percentual glicêmica nos diferentes intervalos de tempo.

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Obtenção de um encapsulado usando berry nativa amazônica para aumentar a bioacessibilidade e bioatividade após digestão simulada in vitro

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Palavras Chave:*Antocianinas,Bioacessibilidade,Digestão,Encapsulação,Produto funcional*

Highlights

Um extrato rico em antocianinas foi encapsulado utilizando maltodextrina e goma arábica.
O encapsulamento aumentou a capacidade antioxidante após digestão*in vitro*.

Resumo/Abstract

A bacabinha (*Oenocarpus minor*), fruta nativa brasileira ainda não amplamente explorada, é rica em compostos fenólicos, principalmente antocianinas e possui alto potencial antioxidante. Entretanto, a instabilidade de fenólicos diante diversos fatores como temperatura e pH, afeta sua bioacessibilidade e bioatividade. Sendo assim, uma alternativa para torná-los menos susceptíveis a estes parâmetros é a microencapsulação. Portanto, esse trabalho teve como finalidade a obtenção e análise dos efeitos da microencapsulação (MENC) de extratos fenólicos (FEN) de*O. minor*, utilizando maltodextrina (MD) e goma arábica (GA), após a digestão simulada*in vitro*pelo método INFOGEST 2.0. Visualmente, os pós apresentaram uma coloração rosa (Figura 1), o que pode evidenciar a presença de antocianinas em sua composição, apesar de terem tons distintos conforme o teste colorimétrico. A microscopia eletrônica de varredura mostrou a presença de formas e tamanhos não padronizados, com bordas irregulares e pontiagudas. O perfil fenólico por espectrometria de massas mostrou aumento de quercetina (*m/z*303) e quercetina-3-O-arabinofuranosídeo (*m/z*435) em MD, enquanto que para GA a tendência foi apenas para epigalocatequina-3-galato na fração digerida. Quanto ao teor de compostos bioativos, a MENC promoveu a proteção dos FEN, apresentando quase 5 vezes mais no MD e GA digeridos. Já as antocianinas apresentaram maior teor para o extrato encapsulado com MD, digerido ou não. Quanto à capacidade antioxidante por ABTS e ORAC, a encapsulação sozinha não foi eficaz em proteger os compostos, mas quando esses pós foram digeridos, a CAOX aumentou. Em suma, os pós encapsulados apresentaram características físico-químicas favoráveis à utilização como ingredientes alimentícios, apresentando FEN e potencial antioxidante mesmo após a digestão. Esses avanços ampliam o potencial tecnológico e a aplicação comercial de ingredientes funcionais à base de extrato de*O. minor*.



Fig. 1- Pós obtidos após o encapsulamento com maltodextrina (a) e goma arábica (b).

Optoelectronic tongue with smartphone-based colorimetry for quality control of cachaças.

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Palavras Chave:*: Cachaça,quality control,optoelectronic tongue,colorimetric sensor array,smartphone*

Highlights

Smartphone-based optoelectronic tongue for cachaça quality assessment; Digital image photometry combined with PCA for classification; Simple and low-cost alternative for quality control of cachaças.

Resumo/Abstract

Cachaça is the most consumed distilled beverage in Brazil and the fourth most consumed worldwide, with high cultural, social, and economic relevance, generating over US$ 20 million in exports annually. Consequently, quality control is essential and official methods rely on gas chromatography, which is time-consuming and requires skilled analysts. To overcome these limitations, an optoelectronic tongue was developed for the discrimination of cachaças samples. The colorimetric array encompasses five chemoresponsive reagents selected to target key quality parameters, 0.2 mmol L^{-1} bromocresol green for acidity; 0.3 mmol L^{-1} phenolphthalein plus 5 mol L^{-1} NaOH for alcohol content; Folin-Ciocalteu reagent for phenolic compounds; 0.2 mol L^{-1} hydroxylamine/10 mmol $L^{-1}Fe^{3+}$ for esters, and Schiff reagent for aldehyde content. Measurements were performed using digital image photometry with a smartphone camera, with color information converted to RGB numerical data. Commercial samples from different origins were analyzed and the results were compared to those obtained by the official method. Principal Component Analysis explained 80% of the total variance, identifying a fingerprint for each group, enabling clear distinction between conform samples and those adulterated by dilution or the addition of acetic acid, acetaldehyde, ethyl acetate, and ethanol. Control charts were defined based on responses to limit concentrations of the main parameters, providing a practical approach for discrimination within the legal limits. The proposed method achieved 100% classification accuracy for 60 commercial samples and 92% for adulterated samples, demonstrating that it is a reliable, low-cost, and promising alternative for cachaça quality assessment. Moreover, accurate results (versus GC-FID) were obtained for the determination of ethanol, acidity, and esters.

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QSPR Modelling for the Prediction of Maximum Absorbance in Novel Organic Food Colourants

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Palavras Chave:*Food Folorings, QSPR, Maximum Absorbance, Virtual Screening,Food Folorings,QSPR,Maximum Absorbance,Virtual Screening*

Highlights

The QSPR model predicts maximum absorbance of organic dyes. Virtual screening of anthocyanins agrees with experimental trends. The model supports rational design and selection of food dyes.

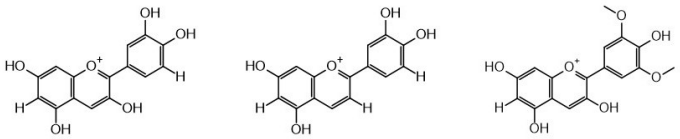
Resumo/Abstract

Food colourants are essential additives used to impart or restore colour, significantly influencing consumer acceptance. However, natural pigments often lack stability, while synthetic azo-compounds raise toxicity concerns. As regulatory standards become stricter, identifying safe alternatives is a vital challenge. In this context, in silico tools offer an efficient pathway to accelerate the discovery of safe compounds. This study develops a Quantitative Structure-Property Relationship (QSPR) model to predict the maximum absorbance of organic colourants. The database comprised 39 structures approved by ANVISA, EFSA, and FDA, partitioned into training and testing sets (80/20). A linear regression algorithm selected six 2D and 3D molecular descriptors, including max_conj_path, nArOR, and WHALES10_Rem. The descriptors highlight the bathochromic effect of increased conjugation and donor groups, while penalising non-compact geometries. The model achieved high statistical performance, with a Training coefficient (R^2) of 0.91, Internal Validation (Q^2) of 0.84, and External Validation (P^2) of 0.71. Error metrics included a Training Mean Absolute Error (MAE) of 14.75 and Root Mean Square Error (RMSE) of 19.50. External validation yielded an MAE of 22.83 and RMSE of 35.00. Virtual screening of anthocyanins, which experimentally range from 465 nm to 550 nm, resulted in predicted values between 451 nm and 544 nm. These results confirm the model's reliability as a screening tool for the rational design and selection of food colourants prior to experimental testing.

Table 1: Statistical performance metrics of the developed linear QSPR model for training, internal validation, and external validation sets.

Training			Internal Validation			External Validation		
R^2	MAE	RMSE	R^2	MAE	RMSE	R^2	MAE	RMSE
0.91	14.75	19.50	0.84	19.69	25.94	0.71	22.83	35.00

Figure 1: Chemical structures of representative anthocyanins selected for virtual screening. The values represent a comparison between experimental data and model predictions for maximum absorbance λ_{max} in nm,



Cyanidin
Prediction: 491 nm
Experimental: 506 nm

Luteolinidin
Prediction: 477 nm
Experimental: 486 nm

Malvidin
Prediction: 519 nm
Experimental: 534 nm

Statistical metrics of linear QSPR model and anthocyanin comparing experimental and predicted λmax.

Agradecimentos/Acknowledgments

The authors thank the KNIME Team, FAPITEC/SE, CAPES, and CNPq for their essential support, provision of research grants, and the computational resources that enabled the development of this study.

Rapid screening for detecting methanol adulteration in distilled beverages using Raman spectroscopy and chemometrics

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Palavras Chave:*Distilled Beverage, PLS, MCR-ALS, Forensic analysis*

Highlights

PLS and MCR-ALS effectively quantified methanol in distilled beverages

MCR-ALS required fewer calibration samples and enabled quantification of the analyte in the presence of unmodeled interferences

Resumo/Abstract

Methanol can be present in alcoholic beverages as a by-product of fermentation or through deliberate adulteration. Due to its high toxicity, reliable and rapid screening methods for the detection and quantification of this alcohol are essential to ensure consumer safety. In this study, Raman spectroscopy combined with chemometric methods was used for this purpose. Different types of distilled beverages were adulterated with methanol, totaling 340 samples. Raman spectra were acquired using a compact Anton Paar Cora 5001 spectrometer equipped with a 1064 nm excitation laser and were preprocessed using standard normal variate. Partial least squares (PLS) and multivariate curve resolution with alternating least squares (MCR-ALS) were used to quantify methanol. Figures of merit, including the root mean square errors of calibration (RMSEC) and prediction (RMSEP), the limits of detection (LOD) and quantification (LOQ), and the correlation coefficient between measured and predicted values (R) were calculated for both models and are shown in Table 1. Although MCR-ALS yielded higher RMSEC and RMSEP, it offers several advantages over PLS, including the demand for fewer calibration samples and the ability to quantify analytes in the presence of interferences not included in the calibration set. Moreover, MCR-ALS model provided not only quantitative information, but also spectral information, allowing recovery of the pure spectra of mixture components. Methanol and ethanol spectra were successfully recovered, with correlation coefficients of 0.903 and 0.934, respectively, compared to the original spectra. The results confirmed that Raman spectroscopy combined with chemometric tools provided an effective and rapid screening strategy for methanol analysis, particularly for detecting alcoholic beverage adulteration.

Table 1. Figures of merit for calibration models.

Model	N_{train}/N_{test}	R	RMSEC (% v/v)	RMSEP (% v/v)	LOD (% v/v)	LOQ (% v/v)
PLS	27/ 313	0.992	1.03	1.17	4.44	13.4
MCR-ALS		0.985	2.53	2.03	2.19	7.22

Agradecimentos/Acknowledgments

CAPES, CNPq, Rede Mineira de Ciências Forenses FAPEMIG, PPGQUI/UFMG, INCTBio-LK.

Spatial–Spectral Characterization of Specialty Coffees Using Near Infrared Hyperspectral Imaging

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Palavras Chave:*Hyperspectral imaging,food chemistry,specialty coffee*

Highlights

NIR hyperspectral imaging enabled differentiation of specialty and common Coffea arabica coffees. Pixel-level modeling significantly improved classification compared to average NIR spectra models.

Resumo/Abstract

The specialty coffee market is expanding, driven by demand for high-quality coffees with superior sensory attributes. Specialty classification requires sensory evaluation (cupping) performed by certified panelists; however, this process is labor-intensive and costly, limiting its suitability for large-scale screening. Consequently, analytical tools capable of supporting preliminary identification of specialty coffees are of considerable interest. Coffee differentiation using near-infrared (NIR) spectroscopy has been widely investigated, particularly for species and geographical origin. Conventional NIR spectroscopy provides rapid chemical information but lacks spatial resolution, as spectra are typically acquired as bulk averages, restricting the evaluation of intra-sample heterogeneity. In contrast, NIR hyperspectral imaging (NIR-HSI) combines spectral and spatial information, enabling pixel-wise chemical assessment and expanding the analytical potential for coffee characterization. In this study, NIR-HSI (900–1700 nm) was applied to classify*Coffea arabica*samples comprising 15 common coffees (CA) and 15 specialty coffees (SA) from different producers in Minas Gerais, Brazil. Principal component analysis (PCA) of mean spectra revealed partial grouping between CA and SA samples. A partial least squares discriminant analysis (PLS-DA) model built using average spectra (66% training set) achieved 64% precision for SA and 88% for CA. To better exploit spatial variability, 100 random pixels per image were extracted for model development, resulting in 95% precision for SA and 91% for CA. Variable importance in projection (VIP) analysis indicated that spectral regions associated with key coffee compounds were more relevant in the pixel-based model. These findings highlight the relevance of incorporating spatially resolved spectral information and support the potential of NIR-HSI as a complementary analytical approach for large-scale pre-screening of specialty coffees.

Agradecimentos/Acknowledgments

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Use of Titanium Dioxide (TiO_2) as a Food Additive in Processed Products: Toxicological Evidence and Regulatory Implications.

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Palavras Chave:*Titanium dioxide,E171,Genotoxicity,Food additives,Food safety regulation.*

Highlights

A literature review on the use of titanium dioxide (E171) in food, addressing toxicological evidence, potential genotoxicity, and regulatory differences between Brazil and the European Union.

Resumo/Abstract

Titanium dioxide (TiO_2), identified in foods as INS 171 or E171, is an additive widely used in the food industry due to its whitening and opacifying properties, being common in ultra-processed products, especially in the confectionery sector. Despite its historical use, E171 has been the subject of increasing scientific and regulatory debate due to uncertainties regarding its toxicological safety, particularly related to the potential genotoxicity of its particles, especially under chronic exposure. In this context, a significant regulatory divergence is observed: while the European Union has adopted restrictive measures culminating in the ban of E171 in foods, based on evaluations by the European Food Safety Authority (EFSA), in Brazil the additive remains authorized in certain food categories. The present study consists of a bibliographic review. A search was conducted in the CAPES database (https://www.periodicos.capes.gov.br/) and SCOPUS (https://www.scopus.com/sources) using the keywords "titanium dioxide (TiO_2)" and "food additive," and the analyzed studies were published between 2015 and 2025, in addition to opinions and legislation from national and international regulatory agencies, such as the European Food Safety Authority (EFSA) and the Brazilian National Health Surveillance Agency (ANVISA). Relevant publications addressing toxicological, genotoxic, and regulatory aspects of titanium dioxide in foods were selected, prioritizing recent studies with greater scientific impact. The analyzed studies indicate that the potential adverse effects of TiO_2 are associated with factors such as particle size, concentration, and exposure time, often related to mechanisms of oxidative stress and damage to genetic material. Thus, the synthesis of the available evidence reinforces the need for caution in risk assessment and for updated discussions within the scope of health surveillance and public health protection in the Brazilian context.



Figure 1. Product label containing E171.

Agradecimentos/Acknowledgments

IFCE – Campus Aracati

Valorização de plantas alimentícias não convencionais a partir do teor de elementos essenciais

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Palavras Chave:*Plantas alimentícias não convencionais (PANCs), Dietas à base de vegetais, Elementos essenciais, Solventes eutéticos profundos (DES), Espectrometria atômica.*

Highlights

PANCs showed relevant Cu, K, Mg, Mn and Zn contents. Caruru stood out, reaching nearly 600% of Mg DRI per 100 g. These plants are promising mineral sources for plant-based diets.

Resumo/Abstract

Plantas alimentícias não convencionais (PANCs) representam alternativas promissoras para a diversificação alimentar e para a promoção de dietas à base de vegetais, porém informações sobre sua composição mineral ainda são limitadas. Este trabalho teve como objetivo avaliar o potencial nutricional de almeirão (Lactuca canadensis L.), caruru (Amaranthus spp.), serralha (Sonchus oleraceus L.) e trapoeraba-roxa (Tradescantia purpurea) quanto aos teores de Cu, K, Mg, Mn e Zn. As amostras foram secas, moídas e submetidas à extração utilizando um solvente eutético profundo (DES) composto por cloreto de colina, ácido málico e água (1:1:10). A extração foi realizada sob condição previamente otimizada, empregando 1,84 g de DES e aproximadamente 0,10 g de amostra, a 60 °C por 30 min, com posterior determinação elementar por ICP OES. Os resultados evidenciaram diferenças expressivas entre as espécies avaliadas. Para o almeirão, observaram-se Cu ≈ 0,10, K ≈ 1137, Mg ≈ 37, Mn ≈ 0,57 e Zn ≈ 0,49 mg/100 g (planta in natura). O caruru apresentou Cu ≈ 0,60, K ≈ 1730, Mg ≈ 737, Mn ≈ 2,3 e Zn ≈ 2,9 mg/100 g. A serralha apresentou Cu ≈ 0,31, K ≈ 620, Mg ≈ 56, Mn ≈ 0,67 e Zn ≈ 2,1 mg/100 g. Para a trapoeraba-roxa, os teores foram Cu ≈ 0,03, K ≈ 165, Mg ≈ 76, Mn ≈ 2,2 e Zn ≈ 1,5 mg/100 g. Considerando uma porção de 100 g, as PANCs avaliadas podem contribuir, em geral, com valores superiores a 30% da ingestão diária recomendada (DRI) para alguns minerais, destacando-se o Mg no caruru, com contribuições que se aproximam de 600% da DRI. Ressalta-se, entretanto, que estudos de bioacessibilidade são necessários para estimar a fração efetivamente liberada no trato gastrointestinal durante a digestão. Os resultados reforçam o potencial dessas PANCs como fontes complementares de minerais em dietas baseadas em vegetais e contribuem para sua valorização e inclusão em sistemas alimentares mais diversos e sustentáveis.

Agradecimentos/Acknowledgments

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49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

CAT - Catálise

Acid Site Chemistry in Hierarchical Zeolites for Heavy Oil Pyrolysis

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Palavras Chave:*Nanozeolites,Acid-site chemistry,Catalytic cracking,Hierarchical porosity,Kinetics*

Highlights

Brønsted acid sites in nanozeolites drive cracking of heavy hydrocarbons
Lewis acid sites enhance selectivity and reducing coke formation
Optimized acidity and accessibility for heavy oil pyrolysis

Resumo/Abstract

The catalytic pyrolysis of heavy oil over hierarchical systems combining nanozeolites with mesoporous materials (MCM-41 and SBA-15) was investigated to elucidate the interplay between acid-site chemistry, mass transport, and kinetic behavior. Nanozeolites provide strong Brønsted acid sites that promote hydrocarbon cracking via carbocation mechanisms, while mesoporous structures enhance accessibility for bulky molecules and reduce diffusion limitations. Kinetic analysis using model-free isoconversional methods (FWO) showed a significant decrease in apparent activation energy (E_a) compared to thermal pyrolysis. The non-catalytic process exhibited $E_a \approx 213$ kJ·mol^{-1}, whereas catalytic systems reduced this value to 142 kJ·mol^{-1} for zeolite HY, 168 kJ·mol^{-1} for MCM-41, and 155 kJ·mol^{-1} for SBA-15. These reductions indicate facilitated reaction pathways due to improved transport and accessibility of active sites. Catalytic systems also shifted conversion to lower temperatures, achieving high conversion at 450–500 °C, compared to above 550 °C for the thermal process. SBA-15 showed superior performance relative to MCM-41, attributed to its higher structural stability and more efficient mass transport, which limit secondary reactions and coke formation. Product distribution at 550 °C confirmed the benefits of hierarchical catalysis, with gasoline yields reaching 40–48 wt%, compared to 26 wt% for thermal cracking. Coke formation decreased from 27 wt% to 16–17 wt% in catalytic systems. This behavior is associated with enhanced diffusion, reduced residence time of intermediates, and improved selectivity. Strong Brønsted acid sites drive cracking and aromatization, while Lewis sites contribute to intermediate stabilization. These results demonstrate that combining nanozeolitic acidity with mesoporous transport networks effectively improves catalytic performance for upgrading of heavy oil into valuable fuels.

Agradecimentos/Acknowledgments

Financial support from the National Council for Scientific and Technological Development (CNPq, Project No. 407460/2025-0), the Brazilian National Agency of Petroleum, Natural Gas and Biofuels (ANP), FINEP and CAPES.

A Practical Kinetic Approach for Extracting Rate Constants in Catalytic Systems with Induction Periods.

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Palavras Chave:*catalytic kinetics, induction period, rate constant, data modeling, homogeneous catalysis,catalytic kinetics,induction period,rate constant,data modeling,homogeneous catalysis*

Highlights

- Reliable rate constants from kinetic curves with induction periods
- Simple and transferable kinetic model for catalysis studies

Resumo/Abstract

Kinetic analyses of catalytic reactions often assume an immediate steady-state regime. However, many homogeneous systems exhibit induction or activation periods related to pre-catalyst transformation or catalyst speciation, leading to deviations from classical first-order kinetics and unreliable rate constants.

In this work, the$X_{mo}d_{el}$ (Fig.1), an induction–growth kinetic model, is introduced for extracting apparent rate constants from catalytic reactions with induction periods. The methodology is illustrated using the solvent-free dehydrogenation of formic acid (HCOOH → H_2 + CO_2) catalyzed by ruthenium complexes. The evolution of gaseous products (H_2 + CO_2) was monitored by water displacement, and the reaction progress was expressed in terms of the conversion fraction, defined as X = Vd/VT, where Vd is the displaced gas volume at time*t*and VT is the theoretical total volume corresponding to 100% conversion.

The kinetic profiles were analyzed using a delay-plus-first-order formalism ($X_{mo}d_{el}$), defined by two-time regimes depending on the induction time τ. For*t*≤ τ,$X_{(t)}$ = 0, whereas for*t*> τ,$X_{(t)}$ = 1 − exp[−*k*(*t*− τ)], where*k*is the apparent rate constant. Model parameters (τ and*k*) were obtained by global fitting of the full kinetic curve through minimization of the residual sum of squares, $\sum_i[X_i - X_{mo}d_{el}(t_i; \tau, k)]^2$, using nonlinear regression (Excel Solver, GRG Nonlinear), with physically meaningful constraints on τ and*k*.

The$X_{mo}d_{el}$ formalizes induction and growth regimes within a single analytical expression, uses conversion fraction as a universal kinetic variable, enables global fitting of complete reaction profiles, and provides a transparent and easily implementable protocol in homogeneous catalysis.

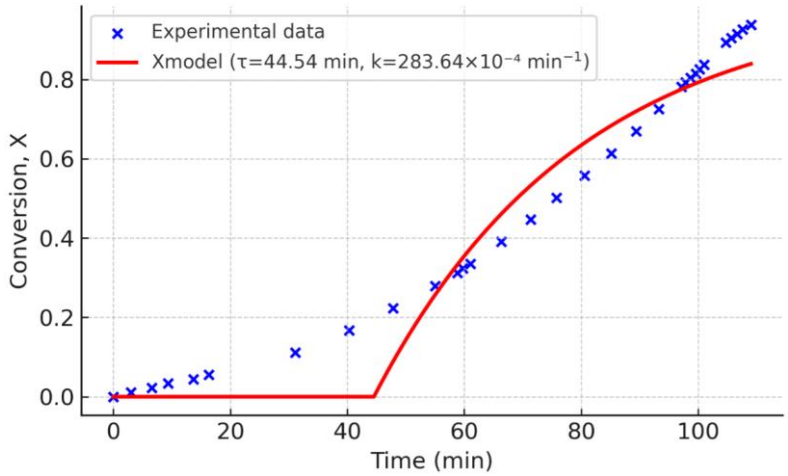


Fig.1: H2 + CO2 evolution (blue points) and the fitted curve using the Xmodel (red line) at 60 °C.

Agradecimentos/Acknowledgments

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BERÇÁRIO DE STARTUPS DA PG-QUÍMICA/UFMG: UM PROJETO DE PRÉ-INCUBAÇÃO PARA ESTIMULAR EMPREENDEDORISMO DE BASE TECNOLÓGICA PARA QUÍMICOS

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Palavras Chave:*Empreendedorismo científico, Startups acadêmicas, Transferência de tecnologia, Inovação, Universidade*

Highlights

University-based program bridges research and market; Academic startup nursery strengthens scientific entrepreneurship; Early-stage support reduces risks in deep tech ventures

Resumo/Abstract

O Berçário de Startups, do Departamento de Química da Universidade Federal de Minas Gerais, é uma iniciativa institucional criada no planejamento estratégico de 2025 do Programa de Pós-Graduação em Química. Este trabalho tem como objetivo, apresentar a estruturação e os resultados iniciais do ambiente de pré-incubação acadêmica e estimular o empreendedorismo científico no Departamento.

O Berçário conta com um programa baseado em 5 fases: (1) Diagnóstico (Análise da Oportunidade), (2) Estruturação da Startup, (3) Lançamento da Startup, (4) Realização de Vendas e (5) Busca por Investidor. Nesta primeira edição (2025/2), o Programa 1 – Diagnóstico (Tabela 1), terá duração de três meses e carga horária total de 15 horas de mentorias, distribuídas em cinco módulos: dor e solução, diagnóstico de mercado, viabilidade econômica, barreiras regulatórias e consolidação tecnológica, com avaliação do Nível de Maturidade Tecnológica (TRL).

A seleção das startups ocorreu por meio de uma divulgação interna e formulário online. Foram submetidas 13 propostas, todas do Departamento de Química da UFMG, das quais 12 foram aprovadas após avaliação por Comitê Gestor, considerando critérios de potencial inovador, clareza da proposta, alinhamento institucional e maturidade tecnológica. As startups selecionadas têm predominância nos níveis TRL 3 a TRL 6, e atuam em áreas como materiais avançados, energia, biocombustíveis, bioeconomia, sustentabilidade, educação científica, tecnologias digitais, química forense e economia circular.

Espera-se como resultado, um modelo viável e eficaz de pré-incubação acadêmica, que promova a formação empreendedora de pesquisadores e fortaleça a interface universidade–mercado, com potencial de consolidação como instrumento estratégico de inovação no ambiente universitário.

Tabela 1. Módulos e conteúdos do Programa 1 – Diagnóstico (Análise da Oportunidade)

Módulo	Carga Horária	Conteúdo
1. Dor e Solução	2H	Identificação das dores e clientes potenciais;
		Definição das soluções tecnológicas;
		Elaboração do Mapa da Empatia;
		Construção do Canvas de Proposta de Valor.
2. Diagnóstico de Mercado	4H	Estruturação do modelo de negócios;
		Descrição da cadeia produtiva;
		Estimativa da dimensão do mercado;
		Mapeamento de concorrentes.
3. Viabilidade Econômica e Mercadológica	6H	Cálculo de custos de produção e precificação;
		Análise de OPEX e CAPEX;
		Avaliação preliminar de investimento e retorno.
4. Potenciais Barreiras	2H	Identificação de barreiras legais, logísticas, ambientais e regulatórias.
5. Finalização Tecnológica	1H	Consolidação das informações e validação final da oportunidade tecnológica.

Tabela 1. Módulos e conteúdos do Programa 1 – Diagnóstico (Análise da Oportunidade)

Agradecimentos/Acknowledgments

Agradecemos às instituições de fomento FAPEMIG, CAPES, CNPq, ESCALAB, Departamento de Química e ao Programa de Pós-Graduação em Química da UFMG.

Bimetallic and trimetallic layered double hydroxides as potential catalytic systems for CO2 conversion

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Palavras Chave:*Layered double hydroxides,Bimetallic,Trimetallic,CO2 conversion*

Highlights

The conversion of CO_2 into epoxides using a potential catalytic system involving new Shigaita-type double lamellar hydroxides (HDLs), with bimetallic and trimetallic phases, was tested.

Resumo/Abstract

Carbon dioxide (CO_2), a greenhouse gas mainly emitted by anthropogenic activities, can be sustainably valorized through cycloaddition reactions that produce value-added products such as cyclic carbonates, which require catalysts, with layered double hydroxides (LDHs) standing out as efficient and low-cost alternatives. New Shigaite-like LDHs are represented by the general formula $[M^{2+}{}_6Al_3(OH)_{18}][B^+(H_2O)_6(SO_4)_2]\cdot 6H_2O$ (B^+ = Li, Na or K) and remain unexplored, as their syntheses have only recently been reported. Therefore, this study aimed to evaluate Shigaite-like LDHs as catalysts for CO_2 cycloaddition into epoxides reactions, comparing bimetallic phases (Zn_6Al_3 and Ni_6Al_3) and a trimetallic phase ($Zn_3Ni_3Al_3$). For the synthesis of the compounds, 1 mol L^{-1} KOH solutions were added to an aqueous solution containing K_2SO_4, $Al_2(SO_4)_3$, and $M^{2+}SO_4$ salts until the pH 8. The resulting solids were separated by centrifugation, redispersed, washed several times, and dried at 40 °C for 72 h. X-ray diffraction (XRD) patterns indicated that all compositions exhibited a basal spacing close to 11 Å, typical of LDHs intercalated with SO_4^{2-} in a double-layer arrangement in the presence of hydrated K^+. Inductively coupled plasma optical emission spectrometry (ICP-OES) analyses confirmed that the phase compositions were very close to the nominal values. CO_2 cycloaddition reactions performed in the absence of tetrabutylammonium bromide (TBAB) led to very low product formation, preventing reliable quantification for the bimetallic LDH samples; under these conditions, detectable product formation was observed only for the trimetallic LDH. Upon the addition of 0.1 mol% TBAB as a co-catalyst, the trimetallic LDH achieved 100% selectivity with a yield of 66.2%. The bimetallic LDHs, in contrast, reached approximately 45% yield while maintaining 100% selectivity. All reactions were carried out at 11 bar of CO_2 and 100 °C for 24 h.Testing with TBAB produced a 29% yield and 100% selectivity.

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Bimetallic catalysis based on Pd/Cu for the preparation of biaryls

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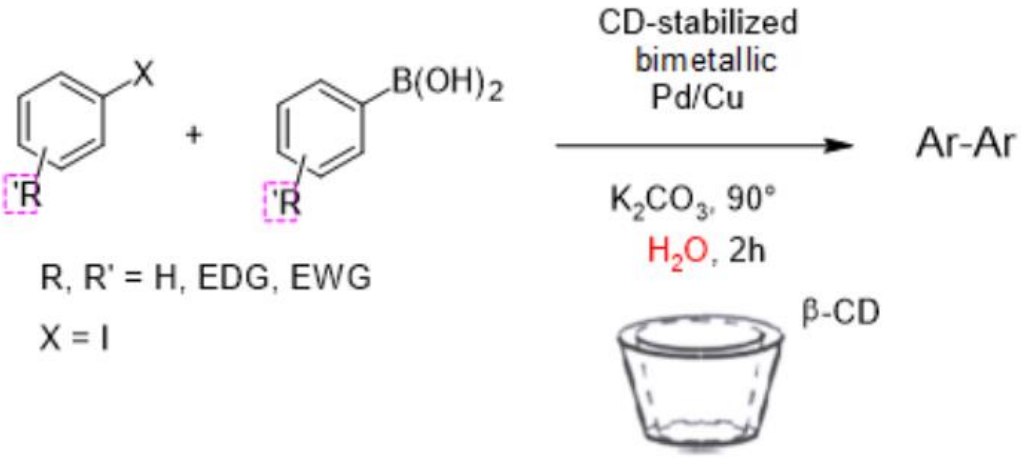
Palavras Chave:*C–C coupling; Bimetallic catalysis; Metal nanostructures; Copper–Palladium; Sustainable chemistry.*

Highlights

Cu–Pd bimetallic systems showed enhanced catalytic performance Possible cooperative metal effects can improve C–C coupling Cyclodextrin as a functional additive for aqueous catalysis

Resumo/Abstract

Biaryl core formation reactions are widely studied given their numerous applications. Despite the existence of consolidated catalytic methodologies, many still rely on the use of pure noble metals, which motivates the investigation of alternatives based on first-row transition metals. In the case of copper, its relative low cost combined with good reactivity requirements that make it a promising alternative (MIYAURA; SUZUKI, 2011; MASTALIR et al., 2024). In this context, this work sought to synthesize and characterize copper and palladium nanostructures by using cyclodextrin(CD) as a reducing and stabilizing agent and Cu/Al layered double hydroxides (LDH) containing Pd(0) as a precursor. The synthesis of the bimetallic dispersion with CD was conducted in aqueous medium with Na_2PdCl_4, $CuSO_4$, and $Pd_2(dba)_3$ precursors. The synthesis of the Cu/Al LDH was carried out according to previous work (NEVES et al., 2017). The catalytic activity was evaluated in the Suzuki-Miyaura model reaction between iodobenzene and phenylboronic acid in water for 2h at 90°C. It was observed that the presence of the bimetallic system (10 mol% Cu; 0,25 mol% Pd) resulted in superior catalytic activity, with conversion and yield values of 100% and 89%, respectively. Control tests showed that the homocoupling reaction was not significantly activated under these conditions (< 5%). UV-vis analysis of the catalytic system indicated the presence of an alternative band at 813 nm, suggesting the formation of a an alloy bimetallic structure (PALMEIRA-MELLO et al., 2021). Studies are underway to evaluate the effect of substituents and electrophiles, as well as the reuse and stability of the catalyst. Additionally, the investigation of catalytic tests using Cu/Al LDH as catalytic precursor.



Representation of the Cu-Pd/Cyclodextrin catalytic system in aqueous medium.

Agradecimentos/Acknowledgments

CNPq, CAPES, SBQ, FAPERJ, GESC

Biogenic synthesis of palladium nanoparticles using ora-pro-nobis extract (Pereskia aculeata): An efficient catalyst for the Suzuki-Miyaura reaction

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Palavras Chave:*biosynthesis, Pd nanoparticles, ora-pro-nobis, catalyst, Suzuki-Miyaura*

Highlights

Obtaining Pd nanoparticles via a biogenic route using an aqueous extract of ora-pro-nobis.

Pd nanoparticles with a diameter of 11 nm and active for up to 10 recycles in the Suzuki-Miyaura reaction.

Resumo/Abstract

Eco-friendly organic synthesis reactions are always sought after, whether through the use of less toxic reagents or the employment of sustainable catalysts. In this sense, obtaining catalysts containing palladium nanoparticles (Pd NPs) via greener routes has aroused interest.[1] Thus, the present work reports the synthesis of Pd NPs via biogenic route using the aqueous extract of*Pereskia aculeata*(ora-pro-nobis). This extract was obtained from fresh leaves of the plant (10 g) crushed with 100 mL of distilled water (pH = 4) and refluxed for 5 h. After filtration, 10 mL of the obtained extract were added to 10 mL of a water/ethanol mixture (1:1) and the pH adjusted to 10. The solution was placed in an ultrasonic bath and received 50 mL of 1 mM $PdCl_2$ solution dropwise, with sonication for 24 h. In this way, Pd(II) cations were reduced with the formation of stable Pd(0) NPs with an average diameter of 11 nm (Figure 1). The isolated Pd NPs (named Pd@OPN) were tested as a catalyst for the Suzuki-Miyaura cross-coupling reaction. Thus, a catalytic system employing phenylboronic acid, aryl halides, Pd@OPN (catalyst, 0.3 mol% Pd), K_2CO_3 (base), ethanol (solvent), N_2 atmosphere, 100 °C and a variable reaction time was adopted to initiate the studies. Several*p*-substituted aryl iodides, containing electron-donating groups, were tested and produced excellent yields (86-99%) in reaction times of less than 12 h. When different aryl bromides were tested, the reaction yields ranged from 38-86% using 20 h of reaction, with the best result (86%) using an ArBr with the CN group in the*para*position (electron-withdrawing group). For aryl chlorides, the worst aryl halides for this reaction, the catalytic system showed poor performance (12-24% yield). The Pd@OPN catalyst showed activity up to the tenth recycle, indicating the robustness and stability of the material.

[1]SN Applied Sciences 2021, 3:243.

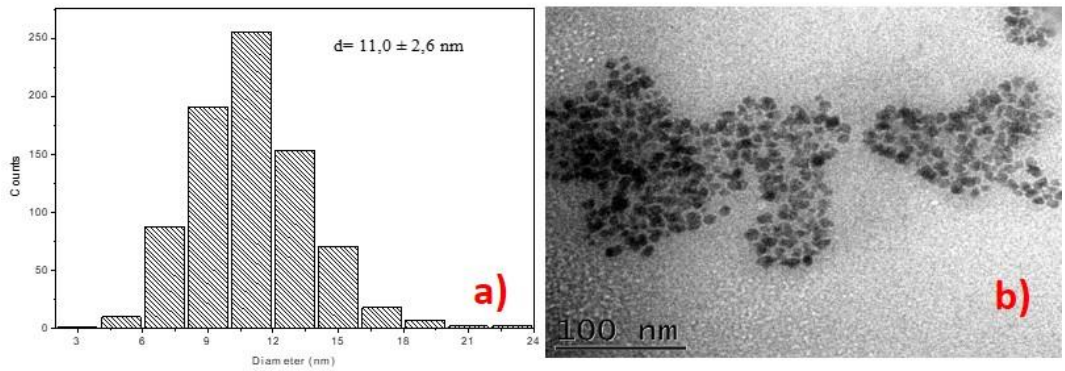


Figure 1. a) Histogram and b) TEM micrograph of Pd NPs.

Agradecimentos/Acknowledgments

C. S. F. thanks CAPES for the doctoral scholarship. The authors also thank the Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (FAPERGS) for funding the research through call for proposals 06/2024.

Biopolymers as reactive platforms for catalytic neutralization of organophosphates: chemical modification and evaluation of neutralizing gels

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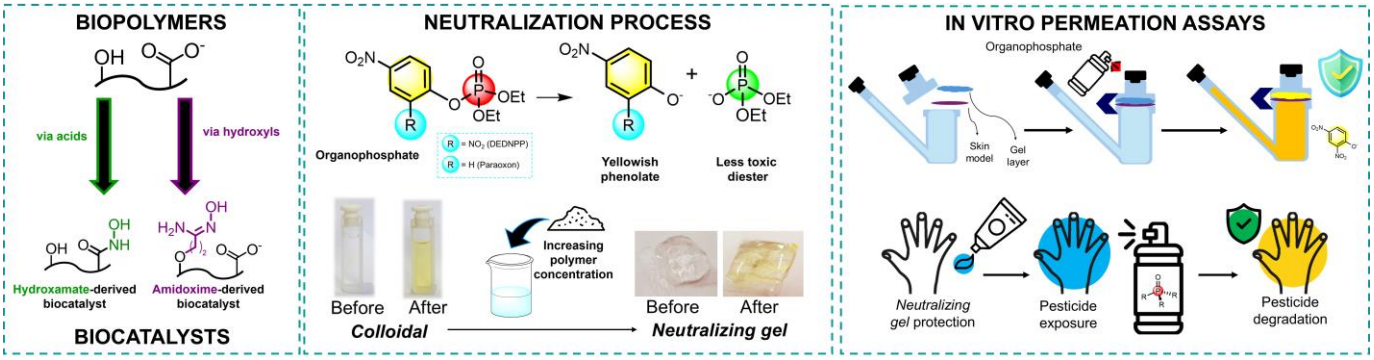
Palavras Chave:*Organophosphate,Catalyst,Alpha-nucleophile,Biopolymer,Gel*

Highlights

Hydroxamate- and amidoxime-functionalized biopolymers with optimized synthesis and formulation enabled efficient catalytic neutralization of organophosphates in colloidal and gel forms.

Resumo/Abstract

Organophosphates comprise neurotoxic compounds usually employed as agrochemicals and chemical warfare agents. Due to their high chemical stability, neutralization processes are very slow and challenging. Alpha-nucleophiles (*e.g.,*hydroxamates and amidoximes) can increase reactivity against organophosphates but commonly lead to non-selective pathways and nucleophile deactivation. Targeted functionalization of these reactive groups onto platforms (such as biopolymers) can modulate and promote efficient catalytic processes: reactive, selective, and recyclable. Herein, we first focused on optimizing the chemical modification of carboxylate groups (into hydroxamates) or hydroxyl groups (into amidoximes) of cellulose derivatives (commercial carboxymethyl cellulose and hydroxypropyl methylcellulose) using mild synthesis conditions. Chemical modification was confirmed by several techniques (*e.g.,*FTIR, CHNS elemental analysis, potentiometric titrations, and TGA). Then, we evaluated the samples as colloidal biocatalysts for neutralization reactions of simulant 2,4-dinitrophenyl phosphate (DEDNPP) and real pesticide Paraoxon, unveiling rate enhancements up to 10^4-fold – among the best in the literature. After that, these biocatalysts were added in different contents to biopolymeric matrices aiming neutralizing gels for organophosphates. The gel samples were characterized by rheology and their reactivity against organophosphates was assessed with*in vitro*permeation assays using DEDNPP, leading to pronounced degradation (up to 80%) after only a few hours. Overall, robust detoxifying agents were achieved in colloidal and gel forms, promoting sustainable, fast, efficient, and affordable biocatalysts for organophosphates, a worldwide concern.



Main points of this work: materials synthesis, neutralization process and in vitro permeation assays

Agradecimentos/Acknowledgments

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Catalisador à base de níquel suportado em carvão ativado para hidrodesoxigenação de compostos fenólicos

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Palavras Chave:*catalisadores à base de níquel,carvão ativado,hidrodesoxigenação*

Highlights

O controle da temperatura de redução ajusta o tamanho dos cristalitos de Ni e maximiza a conversão do fenol.

Resumo/Abstract

A transição energética mundial exige soluções inovadoras como o diesel verde obtido via hidrodesoxigenação (HDO) de óleos vegetais, cuja implementação enfrenta desafios técnicos inerentes à atividade, como estabilidade, conversão e seletividade catalítica. Catalisadores baseados em níquel suportados em carvão ativado (Ni-CA) são promissores para HDO devido ao baixo custo, abundância e estabilidade. Neste estudo a influência da temperatura de redução no desempenho catalítico do Ni-CA em HDO do fenol, molécula-modelo de compostos fenólicos oriundos de biomassa, foi investigado. Os catalisadores Ni-CA foram preparados por impregnação úmida com teores de Ni ~ 5% e reduzidos a 300, 450 e 600 ºC durante 30 min em H_2 (30 mL/min). O CA foi caracterizado por fisissorção de N_2 e porosimetria de Hg, revelando a coexistência de meso- e macroporos, textura ideal para a dispersão metálica. A partir das curvas de TG observou-se alta estabilidade térmica do carvão ativado em atmosfera inerte de N_2 até 1000 ºC, porém em atmosfera oxidante houve completa degradação entre 400-610 °C.**As curvas de H_2-TPR do Ni-CA apresentou picos em: (i) 200 – 300 ºC associada a partículas de NiO maiores fracamente adsorvida no CA; (ii) 400 – 600 ºC atribuído a redução de partículas de NiO menores e com maior interação com o CA. Acima de 600 °C não houve variação do consumo de H_2 indicando inércia do CA nas condições de medida, uma vez que a formação de metano é favorecida sob pressões elevadas (~5 MPa)**.Os difratogramas de DRX confirmaram a formação de níquel metálico, cujo tamanho de cristalito foi influenciado pela temperatura de redução, sendo de 20, 22 e 32nm, nas temperaturas de 300, 450 e 600 ºC, respetivamente. A coexistência de meso- e macroporos e o controle da temperatura de redução são fatores essenciais para obter um catalisador com alto potencial de hidrodesoxigenação, superando as limitações dos suportes tradicionais e constituindo uma rota promissor.

Agradecimentos/Acknowledgments

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Catalytic conversion of CO2 into cyclic carbonates using the ionic liquid (BMI)2[PdCl4]2

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Palavras Chave:*Ionic liquid, CO_2 conversion, Cyclic carbonates,Ionic liquid,CO2 conversion,Cyclic carbonates*

Highlights

Ionic liquid synthesized from BMI·Cl and $PdCl_2$ as a catalyst for the CO_2 cycloaddition reaction to form cyclic carbonates.

Resumo/Abstract

The need for sustainable strategies to reduce CO_2 emissions has encouraged the development of catalytic routes that convert this greenhouse gas into value-added products, with the cycloaddition of CO_2 to epoxides standing out due to its high atom efficiency and mild operating conditions. [1].
In this study, the ionic liquid with a metallic anion, $(BMI)_2[PdCl_4]$, is proposed as a catalyst for CO_2 cycloaddition, exploring its bifunctional nature.
The ionic liquid was synthesized by the direct reaction between BMI·Cl and $PdCl_2$ in a 2:1 molar ratio [2] for 24 h using methanol as solvent, resulting in the formation of the imidazolium metallic salt. After the reaction and methanol removal under reduced pressure, a brown solid was obtained, whose structure was satisfactorily confirmed by single-crystal X-ray diffraction (Figure 1a). The ionic liquid acted as a catalyst for the CO_2 cycloaddition reaction with propylene oxide. The reaction was carried out using 1 mL of epoxide and 0.9485 g of catalyst, under 12 bar of CO_2 at 120 °C for 24 h. The formation of propylene carbonate as the product was confirmed by ^{1}H NMR analysis (Figure 1b), along with the appearance of a signal at approximately 4.7 ppm, attributed to the presence of HDO. Gas chromatography analyses showed that the catalyst exhibited a selectivity of 97.1% toward the cyclic carbonate and a yield of 63.1%.
This study demonstrates that the ionic liquid $(BMI)_2[PdCl_4]$ shows high potential for application as a catalyst in the cycloaddition reaction of CO_2 to epoxides, aiming at the development of a more efficient, robust process aligned with the principles of green chemistry.

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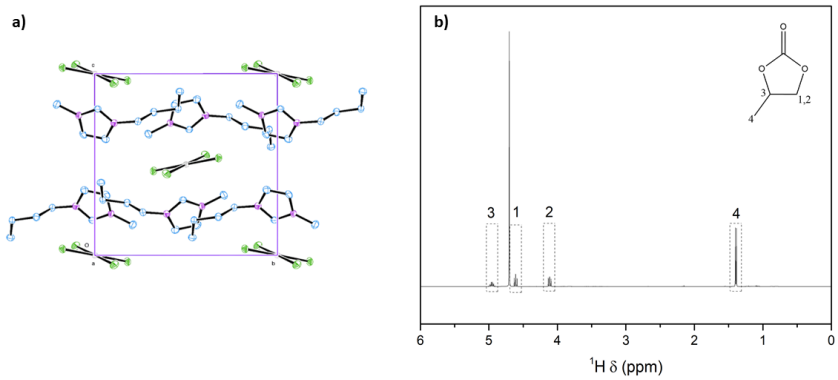


Figure 1: a) Packing of the IL obtained by single-crystal X-ray diffraction; b) ^{1}H NMR spectrum.

Agradecimentos/Acknowledgments

This study was funded in part by CNPq and CAPES. C.W.L. acknowledges the support of Fundação Araucária and SETI through a Research and/or Technological Development Productivity Fellowship.

Catalytic conversion of lignocellulosic carbohydrates over zeolites in a molten salt hydrate medium

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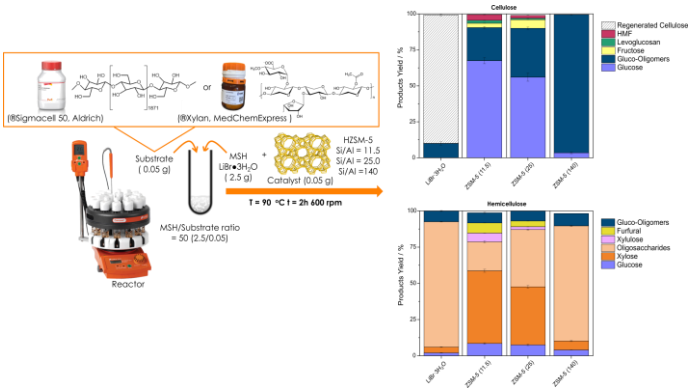
Palavras Chave:*Cellulose,Hemicellulose,Zeolite catalysis,Molten salt hydrate,HZSM-5*

Highlights

Cellulose and xylan dissolve efficiently in LiBr·3H$_2$O under mild conditions.HZSM-5 zeolites promote controlled depolymerization by Brønsted acidity avoiding humins. Si/Al ratio tunes sugar yields.

Resumo/Abstract

Zeolites are versatile solid acid catalysts for biomass conversion. However, their performance is often limited by the poor solubility of lignocellulosic carbohydrates in conventional reaction media. Molten salt hydrates (MSH) provide an alternative reaction environment by dissolving carbohydrates and enhancing contact between macromolecular chains and catalytic acid sites. In this work, well-characterized HZSM-5 zeolites with different Si/Al ratios (11.5, 25 and 140) were evaluated for the catalytic conversion of commercial cellulose and hemicellulose (xylan) in LiBr·3H$_2$O, under mild conditions (90 °C, 2h and 600 rpm). The molten salt hydrate medium enabled complete dissolution of both carbohydrates, and the hydrolysis products distribution was strongly dependent on the zeolite Si/Al ratio (Fig. 1). Monomeric sugars were the main products, with yields reaching up to ~65% and 50% for glucose and xylose, respectively, over HZSM-5(11.5), which exhibits moderate Brønsted acidity (603 µmol g^{-1}). Minor formation (3-7% yield) of by products originated from isomerization and dehydration reactions was also observed. When zeolites with higher Si/Al ratios were used, oligosaccharides were predominantly formed (maximum of 79% yield for Si/Al =140). All HZSM-5 samples exhibited similar textural properties, with specific surface areas around 400 m^2 g^{-1} and pore volumes close to 0.2 cm^3 g^{-1}, while their acidity – comprising both Brønsted and Lewis sites – was governed by the Si/Al ratio. The density of Brønsted acid sites, governed by the Si/Al ratio, controlled glycosidic bond cleavage and secondary dehydration reactions. An adequate balance of acidity favored selective depolymerization while suppressing humin formation and preserving high carbon balance. These results demonstrate that LiBr-based molten salt hydrates combined with acidity-tuned HZSM-5 zeolites constitute an efficient catalytic system for lignocellulosic carbohydrate valorization under mild conditions.



Product distribution from cellulose and xylan conversion in LiBr·3H2O catalyzed by HZSM-5 zeolites.

Agradecimentos/Acknowledgments

The authors acknowledge CNPq (Processes No. 446582/2024-7; 182020/2025-8 and 314796/2025-8) for financial support.

Catalytic Pyrolysis of Petroleum over H-Beta Zeolite: Acid-Site Chemistry, Kinetics, and Product Selectivity

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Palavras Chave:*H-Beta zeolite, Acid-site catalysis, Petroleum cracking, Structure–activity relationship Thermal analysis.,H-Beta zeolite,,Acid-site catalysis,Petroleum cracking,Structure–activity relationship,Thermal analysis.*

Highlights

H-Beta acid sites lower activation energy in catalytic cracking

Zeolite acidity and pores drive selective fuel-range products

Structure–activity links acidity to cracking and coke control

Resumo/Abstract

The catalytic pyrolysis of a petroleum sample over H-Beta zeolite was investigated with a focus on acid-site chemistry and zeolite structure–activity relationships governing hydrocarbon cracking. The H-Beta zeolite, characterized by a three-dimensional channel system with interconnected 12-membered ring pores and a high density of Brønsted acid sites. These features are critical for enhancing cracking selectivity toward light hydrocarbons while limiting excessive coke formation. Thermal and catalytic pyrolysis experiments were carried out from room temperature to 900 °C at heating rates of 5, 10, and 20 °C min^{-1} using a petroleum sample with API gravity of 35.2. Thermogravimetric analysis (TG/DTG) revealed a three-step mass-loss profile associated with volatilization of light compounds, acid-catalyzed cracking of high-molecular-weight aromatic species, and subsequent coke degradation. In the presence of H-Beta zeolite, all degradation steps shifted to lower temperatures, indicating accessibility of reactants to active Brønsted sites and enhanced catalytic efficiency. Product analysis by pyrolysis–gas chromatography–mass spectrometry (Py-GC/MS) at 250, 350, and 450 °C demonstrated that H-Beta zeolite significantly altered the degradation pathway, favoring the formation of gasoline- and diesel-range hydrocarbons over random thermal scission products. Kinetic parameters obtained using the Vyazovkin model-free isoconversional method showed a pronounced reduction in activation energy in the cracking conversion range under catalytic conditions. This reduction reflects the effectiveness of the zeolite acid sites in stabilizing reaction intermediates and lowering energy barriers. Overall, the results establish clear correlations between zeolite acidity, pore architecture, and catalytic performance, highlighting H-Beta zeolite as an efficient catalyst for petroleum cracking and upgrading.

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CdS/ZnO electrospun nanofiber heterostructure for efficient solar-driven hydrogen production

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Palavras Chave:*electrospinning,heterojunction,S-scheme,photocatalytic hydrogen evolution,sonochemical synthesis*

Highlights

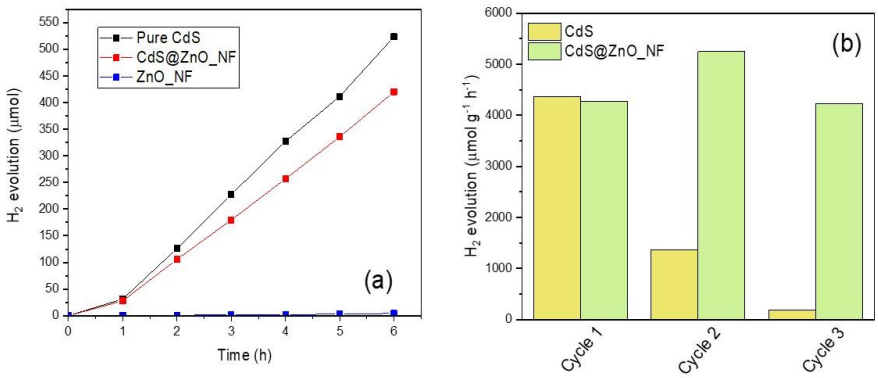
Heterostructure was prepared combining electrospinning and US deposition

CdS@ZnO NFs achieved an exceptional H_2 evolution

The outstanding performance is due to 1D NFs architecture and efficient S-scheme

Resumo/Abstract

Advances in solar-driven hydrogen production rely heavily on the design of photocatalysts that maximize utilization of visible light while minimizing charge recombination. Despite significant progress in semiconductor-based photocatalysis, achieving high efficiency with low CdS loading remains challenging. Here, we introduce a hybrid strategy combining electrospinning and sonochemical deposition to produce a highly efficient CdS/ZnO heterostructure with enhanced activity. Electrospun ZnO nanofibers decorated with CdS nanoparticles (CdS@ZnO NFs) were successfully synthesized via a sonochemical-assisted deposition method and evaluated as photocatalysts for H_2 production under simulated sunlight. Structural, morphological, and spectroscopic analyses confirmed the formation of a well-defined CdS/ZnO heterostructure. Compared with pristine CdS and ZnO NFs, the composite exhibited enhanced optical absorption, favorable band-edge alignment, and more efficient charge separation, as indicated by its superior photocurrent response. The CdS@ZnO NFs achieved an exceptional hydrogen evolution rate of 13.4 mmol g^{-1} h^{-1}, outperforming pristine CdS by more than threefold and surpassing most previously reported ZnO/CdS systems. The composite also demonstrated remarkable photostability over three consecutive cycles, whereas pure CdS rapidly deactivated due to photocorrosion. The enhanced activity and durability are attributed to the one-dimensional nanofibrous architecture and to an S-scheme–like charge-transfer behavior at the CdS/ZnO interface, which promotes effective charge separation while preserving strong redox capability. These results highlight interfacial engineering in CdS/ZnO nanofibers as a promising strategy for developing efficient photocatalysts for solar-driven hydrogen production.



(a) Kinetic curves of hydrogen production for pure CdS, ZnO NFs, and CdS@ZnO NFs. (b) Recycle test f

Agradecimentos/Acknowledgments

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Ciprofloxacin photoelectrochemical degradation over CuWO4|BiVO4 heterojunction

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Palavras Chave:*Electrodeposition,Thin film,Emerging pollutant,Photoelectrocatalysis,Wastewater treatment*

Highlights

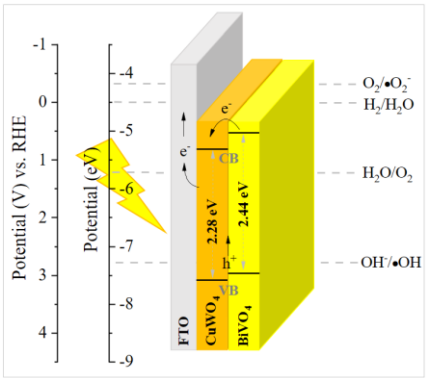
$BiVO_4$ and $CuWO_4$ were synthesized by electrodeposition

$CuWO_4|BiVO^4$ achieved 78% CIP degradation

$CuWO_4|BiVO_4$ exhibited conventional type II charge transfer behavior

Resumo/Abstract

The presence of antibiotics, such as ciprofloxacin (CIP), in wastewater represents a global threat due to the generation of super-resistant bacteria. In this sense, the development of an environmentally efficient system for CIP removal is necessary. Thus, electrodeposition of a $BiVO_4$ and $CuWO_4$ heterojunction was employed in the phot-oxidation of CIP in a photoelectrochemical (EHP) system. Therefore, $BiVO_4$, $CuWO_4$, $BiVO_4|CuWO_4$ and $CuWO_4|BiVO_4$ were investigated using ultraviolet-visible (UV-Vis), photoluminescence (PL), X-ray diffraction (XRD), and photoelectrochemical characterization techniques. Results obtained by UV-Vis indicated absorbance within the visible spectrum. The crystalline of the materials was confirmed by XRD. $CuWO_4|BiVO_4$ showed a reduction in photoluminescence (PL) emission intensity, indicating greater efficiency in charge separation and, consequently, better photocatalytic activity. The junction of these semiconductors enhanced their photoelectrochemical capabilities, as well as decreasing the resistance to charge transfer in the $CuWO_4|BiVO_4$ heterojunction. In linear scan voltammetry, the $BiVO_4$, $CuWO_4$, $BiVO_4|CuWO_4$, and $CuWO_4|BiVO_4$ films exhibited photocurrent densities (applied potential of 0.7 V) of 71 µA, 29 µA, 47 µA, and 133 µA, respectively. This is due to the formation of a type II staggered heterojunction. Based on the energy diagram in Figure, obtained from experimental results, the $CuWO_4|BiVO_4$ heterojunction showed a favorable contribution. In recombination, electrons from the CB of $BiVO_4$ move to the CB of $CuWO_4$, where they are collected by the external circuit, extending the lifetime of the charge carriers. Catalytic tests performed under photolysis, photocatalysis (HP), and EHP conditions demonstrated a more significant degradation under the EHP condition in the $CuWO_4|BiVO_4$ heterojunction, reaching 78% CIP degradation. This demonstrates that the $CuWO_4|BiVO_4$ heterojunction is an excellent proposal for the treatment of pharmaceutical waste.



Energy diagram of the CuWO4|BiVO4 heterojunction

Agradecimentos/Acknowledgments

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Computational assessment of direct CO2 hydrogenation catalyzed by iron porphyrin

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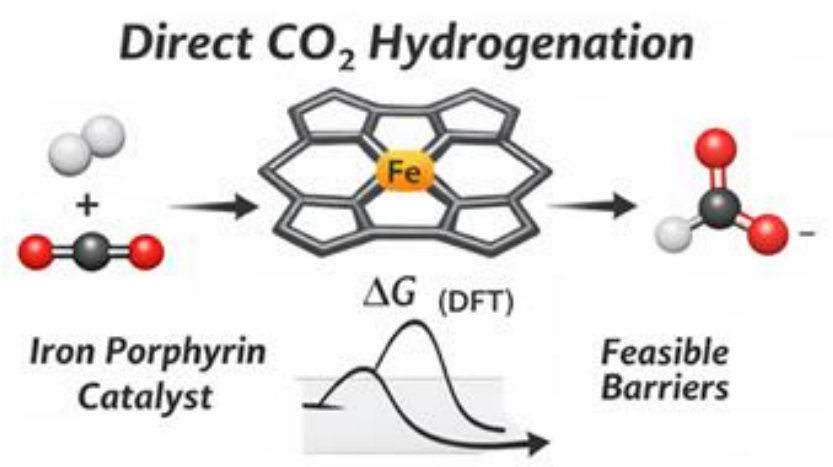
Palavras Chave:*High throughput screening,Olefin Metathesis,Cyclopropanation,Iron,DFT,Carbon Dioxide,Hydrogenation,Iron Porphyrins,Catalysis,DFT*

Highlights

-DFT shows iron porphyrins promote carbon dioxide hydrogenation
-Hydride transfer is the rate determinant step
-Fe(III) lowers barriers
-Base (NEt_3) boosts carbon hydride transfer

Resumo/Abstract

Carbon dioxide (CO_2) emissions drive climate change, necessitating innovative capture and conversion strategies. Catalytic hydrogenation with affordable and abundant catalysts offers a promising solution. Using density functional theory (M06L), we computationally evaluate iron porphyrins as potential promoters of CO_2hydrogenation, focusing on the reaction mechanism and the influence of iron oxidation and spin states. Our analysis reveals that porphyrin systems with Fe^{2+}in the singlet spin state exhibit the most stable hydride formation step. Additionally, the transition state corresponding to the nucleophilic attack of the hydride to the CO_2 (**TS_{45}**)is the rate-determining step, more stable in the quintet spin state. The porphyrin of Fe^{3+} seems to be more efficient as catalyst, with low barriers. Furthermore, adding a base, such as trimethylamine, during CO_2coordination significantly enhances process efficiency by stabilizing an intermediate more effectively than in base-free conditions. Overall, the iron-porphyrins could be used as catalyst to molecular hydrogenation of CO_2.



Hydrogenation of CO2 catalyzed by Fe(II)-prophyrin

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CONVERSION OF FURFURYL ALCOHOL INTO LEVULINIC ACID AND OCTYL LEVULINATE USING DESILICATED BETA ZEOLITES

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Palavras Chave:*Octyl Levulinates,Furfuryl Alcohol,Levulinic Acid,Biolubricants,Desilicated Zeolites*

Highlights

Desilicated zeolites from a commercial sample showed mesopore formation and altered acidity. Liquid-phase reactions confirmed activity and selectivity toward levulinic acid and octyl levulinate.

Resumo/Abstract

With the growing concerns related to climate change, the use of renewable sources has been increasingly explored. Among them, lignocellulosic biomass stands out as an abundant alternative for energy generation and the production of chemical compounds, although it still presents scientific and technological challenges [1]. In this work, the conversion and selectivity toward levulinic acid (LA) and octyl levulinate (OL) in the alcoholysis of furfuryl alcohol (FFA) were evaluated using desilicated beta zeolites to minimize diffusion limitations. Four catalysts were obtained by desilication, varying the concentration of sodium hydroxide (NaOH) (0.1, 0.2, 0.3, and 0.4 mol L^{-1}) at 50 °C for 30 min [2], and were characterized before and after treatment by XRD, XRF, nitrogen physisorption, and NH_3-TPD (Table 1). XRD results indicated changes in the diffraction patterns with increasing NaOH concentration, showing a reduction in peak intensities due to some loss of the crystalline structure of the zeolites. Consistently, XRF analyses showed a decrease in the SAR ratio, while nitrogen physisorption revealed an increase in mesopore volume. NH_3-TPD indicated an increase in total acidity and acid site concentration, along with a decrease in acid strength as the NaOH concentration increased. In liquid-phase reactions, all desilicated zeolites exhibited catalytic activity and selectivity toward LA and OL in the alcoholysis reactions between FFA and octanol at 150 °C (Table 1). The sample treated with 0.2 mol L^{-1} NaOH stood out, reaching a conversion of 94% after 6 h, with selectivities of 16% for LA and 17% for OL, which were higher than those obtained with the parent zeolite, which showed a conversion of 78% and selectivities of 7% for LA and 10% for OL. These results disclosed the positive impact of an hierarchical porous network in beta zeolite in the production of renewable long-chain alkyl levulinates, which are highly demanded in the energy sector.

Table 1 - Relative crystallinity (C_{XRD}), SAR ratio, specific surface area (S_{BET}), mesopore volume (V_{meso}), acid site density (NH_3-TPD), proportion of strong acid sites, furfuryl alcohol (FFA) conversion, and selectivities to levulinic acid (LA) and octyl levulinate (OL)

Catalyst	C_{XRD} (%)	SAR	S_{BET} ($m^2\ g^{-1}$)	V_{meso} ($cm^3 g^{-1}$)	NH_3-TPD (µmol m^{-2})	Strong (%)	X_{FFA} (%)	S_{LA} (%)	S_{OL} (%)
H-Beta 25	100	26	587	0.629	1,27	47	78	7	10
H-Beta 0.1-30	83	22	546	0.742	1,55	45	82	8	10
H-Beta 0.2-30	77	18	612	1.002	2,02	49	94	16	17
H-Beta 0.3-30	79	18	521	0.832	2,17	45	86	12	15
H-Beta 0.4-30	62	16	463	0.756	2,21	44	63	15	14

Agradecimentos/Acknowledgments

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CO2 Valorization via the Reverse Water–Gas Shift over High-Entropy Oxides

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Palavras Chave:*High-entropy oxides,reverse water-gas shift,exsolution,High-entropy materials,catalysis,CO2 valorization,CO2 hydrogenation*

Highlights

Spinel high-entropy oxides enable stable RWGS catalysis
In situ reduction induces reversible metal exsolution
Embedded Co–Ni–Cu nanoparticles boost CO_2 conversion

Resumo/Abstract

Mitigating climate change requires strategies for CO_2 valorization into value-added chemicals or fuels. The reverse water–gas shift (RWGS) reaction (CO_2 + H_2 CO + H_2O) is a key process for syngas production using green H_2, requiring stable and active metal sites [1]. High-entropy oxides (HEOs), composed of five or more metal cations in a single-phase solid solution, are promising catalysts due to their high configurational entropy, enhancing stability [2]. Under RWGS conditions, defects can promote exsolution of reducible metals (Cu, Ni, Co), generating metallic nanoparticles (NPs) embedded in the oxide matrix, creating unique active sites. In this work, spinels HEOs of Cr, Mn, Fe, Ni, Co, and Cu were synthesized via sol–gel route and evaluated as RWGS catalysts. Nanostructured HEOs spinels (~70 m^2/g) were obtained. In situ XRD under H_2 for $CuNiCoCrMnO_4$ showed the evolution of the spinel structure as a function of temperature, with characteristic fcc peaks of metallic NPs at 220°C. The fcc peaks increased with temperature, along with a partial HEO spinel restructuring into a rock salt-type phase. At 460°C, the spinel structure was restored as the principal HEOs phase coexisting with NPs. STEM images revealed a complex nanostructure; after the reducing pretreatment at 500°C, embedded Co–Ni–Cu alloy NPs were observed. Under reaction conditions (CO_2:H_2 = 1:4, T= 400°C), the pristine HEO catalyst showed high and stable CO_2 conversions over more than 250 min on stream. After reducing pretreatment at 500°C, higher activity and methanation were found and associated with the exsolution process and formation of metallic NPs, highlighting the potential of spinel HEOs for CO_2 valorization.

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The authors thank UNICAMP and CNPEM/LNLS for providing the research infrastructure. The authors also acknowledge financial support from FAPESP (Project No. 2024/20597-6), CNPq (311226/2022-1) and CAPES (001).

DA PESQUISA QUÍMICA PARA O MERCADO: DESENVOLVIMENTO E VALIDAÇÃO DE UM CURSO ONLINE DE EMPREENDEDORISMO TECNOLÓGICO PARA A COMUNIDADE QUÍMICA

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Palavras Chave:*Empreendedorismo científico,educação empreendedora,transferência de tecnologia,startups acadêmicas,deeptechs*

Highlights

Online course bridges chemistry research and entrepreneurship; Action research applied to academic innovation education; Practical tools foster science-based startup creation

Resumo/Abstract

A criação de startups de base tecnológica a partir da pesquisa acadêmica em Química enfrenta barreiras, como complexidade técnica, lacunas na formação empreendedora e a escassez de mecanismos de suporte adaptados ao ecossistema universitário, dificultando a transformação de ciência em inovação de mercado. Este trabalho apresenta o desenvolvimento e a validação de um Produto Mínimo Viável (MVP) de um curso online (Figura 1) voltado à capacitação empreendedora de pesquisadores, visando mitigar a lacuna entre a produção científica e o mercado.

A metodologia baseou-se em pesquisa-ação, estruturada em três etapas: diagnóstico, desenvolvimento e validação. Na fase diagnóstica, foram consultados 84 participantes (graduandos, pós-graduandos e docentes) de universidades brasileiras. Por meio da aplicação do Mapa da Empatia e do Mapa da Dor, foi possível perceber que 70% dos respondentes têm interesse em empreender, com dificuldade de 8/10. As principais dificuldades relatadas foram a falta de conhecimento em gestão, burocrático, ausência de redes de apoio e dificuldades de investimento.

Assim, o MVP foi estruturado em duas partes: (i) Despertando o empreendedor dentro de você, voltada à desmistificação e motivação; e (ii) Avaliando o potencial de sua tecnologia, focada em validação de mercado, desenvolvimento de produto, viabilidade técnica e econômica, modelo de negócios, propriedade intelectual e captação de recursos. O curso obteve 62 inscritos, com 34 participantes ativos que validaram a proposta. Os indicadores de satisfação registraram médias superiores a 7,8/10 para clareza e aplicabilidade.

Os resultados demonstram que a educação empreendedora direcionada é uma estratégia para reduzir a distância entre a universidade e o mercado. O curso aumentou a motivação do público, além de fornecer ferramentas para o dimensionamento de mercado e construção de propostas de valor, que apoiam a transformação de ideias em soluções tecnológicas viáveis.



Figura 1. MVP do curso

Agradecimentos/Acknowledgments

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Effects of the reduction of Ni/Beta zeolite catalysts on the hydrodeoxygenation of phenolic compound

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Palavras Chave:*Ni-based catalysts, Beta zeolite, hydrodeoxygenation,Ni-based catalysts,Beta zeolite,hydrodeoxygenation*

Highlights

Reducing Ni-beta under mild conditions improves metal dispersion and decreases Ni particle size. The efficiency of hydrodeoxygenation of phenol can be increased by controlling the reduction of Ni-beta.

Resumo/Abstract

The ongoing energy transition, driven by the gradual replacement of fossil fuels with renewable energy sources, is essential to achieving effective climate governance and greater national autonomy. In this context, hydrotreated vegetable oils (HVO) have emerged as fuel candidates, as they enable significant reductions in pollutant emissions and can be produced from biomass residues. Among the available conversion routes, hydrodeoxygenation (HDO) catalyzed by nickel-based materials is a promising strategy for converting biomass into HVO. Previous studies have investigated the roles of support composition, active site nature, and reaction conditions in determining HDO efficiency. Despite these advances, the influence of the reduction step on HDO efficiency has received comparatively little attention. In this study, we evaluated the influence of the reduction temperature of Ni catalysts supported on Beta zeolites (BEA, Si/Al = 180) on the HDO of phenol, selected as a representative compound for lignin-derived phenolics. Ni-BEA catalysts (~3.5 wt% Ni) were prepared by wet impregnation and reduced under H_2 (30 mL/min) for 30 min between 300 and 600°C, named Ni-BEA-Rx, where x corresponds to the reduction temperature. The conversion of phenol to cyclohexane and the turnover frequency at time zero (TOF_0) performed in a batch reactor (160 °C, 2 h, and 40 atm H_2) followed the decreasing order: Ni-BEA-R450> Ni-BEA-R300> Ni-BEA-R600. These results, together with supplementary characterizations, corroborate our initial hypothesis: High temperatures (>500°C) and long reduction times (3-5 h), as followed by most published studies on this topic, favor the total reduction of Ni, but lead to an increase in the Ni particle size and reduce the metallic dispersion, which decreases the catalytic efficiency. The way in which Ni-based catalysts are reduced strongly influences their catalytic performance in HDO, reinforcing the need to balance reducibility and metal dispersion.

Agradecimentos/Acknowledgments

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Estudo de catalisadores SiO2@Ni1-xCops@SiO2 na reforma seca do biogás

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Palavras Chave:*Catalisador core@shell, Reforma seca do biogás, Níquel-cobalto, Sílica, Gás de síntese,Catalisador core@shell, Reforma seca do biogás, Níquel-cobalto, Sílica, Gás de síntese,Catalisador core@shell,Reforma seca do biogás,Níquel-cobalto,Sílica,Gás de síntese*

Highlights

Efeito sinérgico entre Ni e Co favorecendo a ativação de CH_4 e CO_2 em menores temperaturas
Síntese de catalisador core@shell

Resumo/Abstract

A reforma seca do biogás é um processo catalítico de grande relevância para a conversão de CH_4 e CO_2 em gás de síntese (H_2 + CO), contribuindo para a mitigação de gases de efeito estufa e para a promoção da economia circular. O presente trabalho teve como objetivo o desenvolvimento e a caracterização de um catalisador com estrutura core@shell do tipo $SiO_2@Ni_{1-x}Co_x@SiO_2$, visando aliar uma boa atividade catalítica e estabilidade térmica. O material foi constituído por nanoesferas de sílica sintetizadas pelo método Stöber, recobertas por uma camada ativa de filossilicato de níquel-cobalto obtida por impregnação úmida. A síntese envolveu etapa de calcinação a 700 °C, com taxa de aquecimento de 10 °C/min em atmosfera de ar sintético. A caracterização por difração de raios X confirmou a formação de fases cristalinas de NiO e Co_3O_4, com tamanho médio de cristalito em torno de 15 nm, enquanto análises de redução à temperatura programada evidenciaram a redução escalonada dos metais, com picos característicos a aproximadamente 570 °C para Co e entre 670 e 740 °C para Ni. Ensaios catalíticos indicaram que o catalisador bimetálico apresentou desempenho superior ao sistema monometálico de níquel, além de seletividade estável para H_2/CO próxima de 1:1. O efeito sinérgico entre Ni e Co favoreceu a ativação dos reagentes em temperaturas mais baixas quando comparado a catalisadores contendo apenas níquel. Testes de estabilidade revelaram desativação moderada ao longo de 20 h de operação, atribuída à sinterização parcial das fases metálicas, embora a arquitetura core@shell tenha se mostrado promissora na mitigação desse efeito. Como continuidade do estudo, encontram-se em andamento a definição da melhor proporção entre os metais ativos, bem como as etapas de funcionalização superficial e encapsulação do catalisador mais eficiente, com o objetivo de aprimorar sua estabilidade e desempenho catalítico.

Ethanol Dehydrogenation over Hydrotalcite-Derived Mixed Oxides

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Palavras Chave:*Heterogeneous catalysis Ethanol dehydrogenation, Hydrotalcite-like compounds, Mixed metal oxides, Acetaldehyde,Heterogeneous catalysis,Ethanol dehydrogenation,Hydrotalcite-like compounds,Mixed metal oxides,Acetaldehyde*

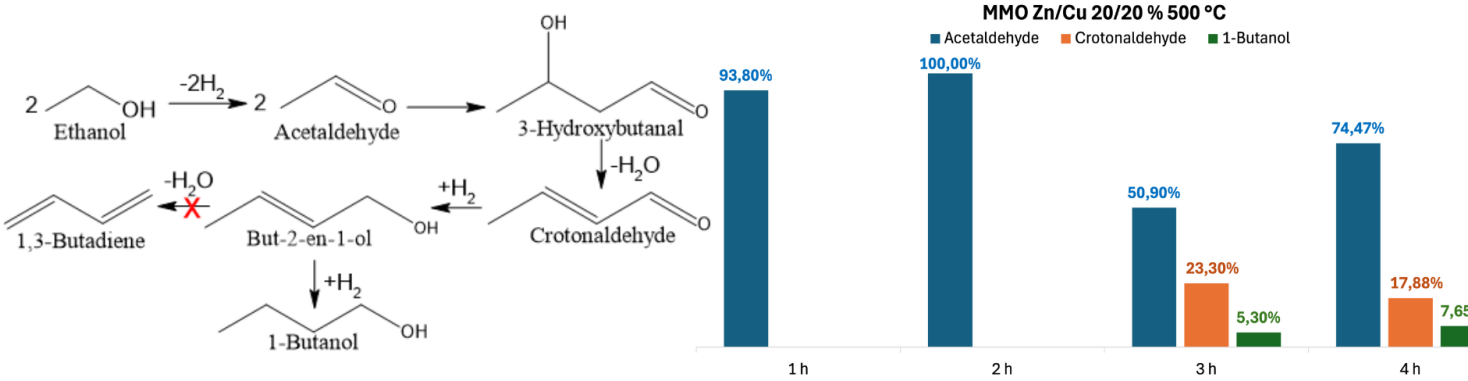
Highlights

Production of acetaldehyde, crotonaldehyde, and 1-butanol via ethanol dehydrogenation.

Hydrotalcite-type catalysts with partial replacement of Mg^{2+} by reactive transition metals.

Resumo/Abstract

The focus on sustainability has been essential in the search for industrial processes based on bio-based feedstocks. With this in mind, the present work aimed to study ethanol dehydration and dehydrogenation routes using hydrotalcite-derived catalysts, partially replacing Mg^{2+} with two reactive transition metals. One of these was Zn^{2+}, selected due to its low carbon deposition, which reduces reactor clogging and catalyst deactivation, combined with other reactive transition metals, Ni^{2+}, Cu^{2+}, and Fe^{2+}.
The reactions were conducted in a low-pressure fixed-bed reactor, with the column packed with each of the mixed metal oxides (10%), 100-200 mesh, and silica gel (90%), 60-100 mesh. The ethanol flow rate was maintained at 0.2 $mL \cdot min^{-1}$, operating temperatures were 400 and 500 °C, and the reactions were carried out for 4 hours. After GC-MS analysis (PerkinElmer Clarus 680® coupled to an MSD 600T) operating in electron impact ionization mode (70 eV, positive mode), it was observed that the catalysts mostly favored the production of acetaldehyde, crotonaldehyde and 1-butanol. Therefore, it is verified that the surface of the synthesized oxides favored ethanol dehydrogenation.
Regarding conversion rates, the catalysts in which Mg^{2+} was partially replaced by Zn^{2+} and Ni^{2+} showed the best performance; at 500 °C, the conversion exceeded 70 %, reaching 95.2 % in the last hour of the reaction. In contrast, the catalysts containing Zn^{2+} and Cu^{2+} exhibited poor performance at 400 °C, with nearly negligible conversion rates of 0.54 % and 2.64 %, respectively. Meanwhile, the Zn^{2+} and Fe^{2+} catalysts showed intermediate results; across both studied temperature ranges, they yielded conversion rates ranging from 31.8 % to 75.8 %. Therefore, the efficiency of the conversion*versus*selectivity system should be further studied, since the selectivity for acetaldehyde does not follow the conversion rate, which is enhanced by the increase in temperature.



Reaction mechanism (left) and product distribution with Zn/Cu 20/20 % MMO at 500 °C (right).

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Evaluation and characterization of CeO2 catalysts synthed via ultrasonic irradiation and applied in CO2 reduction.

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Palavras Chave:*catalysts, conversion, carbon dioxide, methanation*

Highlights

The rise in CO_2 requires sustainable and efficient energy solutions.
The methanation of CO_2 (Sabatier reaction) converts emissions into fuel.
Oxygen vacancies are crucial for catalytic activity.

Resumo/Abstract

The rapid rise in greenhouse gas emissions, especially CO_2, demands sustainable technological solutions. CO_2 methanation (Sabatier reaction) is a promising route because it converts CO_2 and H_2 into CH_4 and H_2O, enabling energy storage and mitigating emissions. This work investigates Ni-based catalysts supported on CeO_2, synthesized by sonoprecipitation, with Y_2O_3 added as a promoter to enhance oxygen vacancy (VO) formation, a key factor for catalytic performance.Catalysts were prepared from metallic salts with pH control and ultrasonic irradiation, followed by drying and calcination. Structural, morphological, and textural properties, as well as oxidation states and VO, were analyzed by XRD, SEM, Raman spectroscopy, and nitrogen physisorption.Even samples produced without sonication showed favorable features for methanation, including good metal dispersion, porous morphology, and intrinsic oxygen vacancies. Y incorporation improved the thermal stability of ceria, increased surface basicity, and mitigated coke deposition. Raman spectra displayed the typical F_2g mode of CeO_2 (~460 cm^{-1}), bands related to oxygen defects (~540–600 cm^{-1}), and signals attributed to NiO. The absence of Ni^0 peaks is consistent with its Raman inactivity. In Y-containing systems, band shifts and broadenings confirmed lattice distortion and additional vacancy generation, while some Y_2O_3 features suggested partial phase segregation.SEM images revealed rough surfaces and homogeneous particle distributions, where smaller particles imply higher surface area and enhanced catalytic potential. XRD confirmed the crystalline fluorite structure of ceria. Peak broadening indicated Y incorporation into the lattice or the presence of highly dispersed Y_2O_3 species. Overall, the CeO_2-Ni-Y_2O_3 combination constitutes a promising catalytic platform. Nickel is the active phase, while ceria acts as a redox support and yttrium as a structural promoter that increases oxygen vacancies and enhances stability

Agradecimentos/Acknowledgments

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Exploring vapor-phase transport routes for the synthesis of macroporous zeolites from silica spheres.

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Palavras Chave:*Zeolites, Vapor-Phase Transport, Macropores*

Highlights

MacMFI zeolite was synthesized using macroporous silica spheres as a template and silica source. The macropores enhance the diffusion of polymer derivatives, which will enable future PLA methanolysis.

Resumo/Abstract

Zeolites are crystalline aluminosilicates that have attracted sustained scientific and industrial interest due to their high surface area, tunable acidity, shape selectivity, and thermal stability[1]. These properties underpin their widespread application as adsorbents, ion exchangers, and catalysts in petrochemical and fine chemical processes[2]. However, the strictly microporous nature of conventional zeolites often imposes severe diffusion limitations, particularly for reactions involving bulky molecules or polymeric substrates[3].

In this work, we explore a vapour phase transport route for the synthesis of MFI-type macroporous zeolites using silica spheres as both sacrificial models and silica sources. Tetrapropylammonium hydroxide (TPAOH) impregnation in the silica beads promotes a vapour phase-assisted recrystallization, whereby the amorphous silica is converted into the MFI zeolitic structure, resulting in hollow macroporous beads with maintained structural integrity. Figure 1a and 1c shows the X-ray diffraction patterns of the solids involved in the process and confirm the successful preparation of MFI-like structure.
By means of the SEM images, it is possible to evidence the disappearance of the spherical silica and the recrystallization of silica into macroporous MFI (Figures 1b and 1c). The morphology of the MFI is somewhat heterogeneous in size but resembles rectangular particles typically observed for this topology. Red circles are included in Figure 1b to show the holes left by the recrystallization under the vapour phase transport route.

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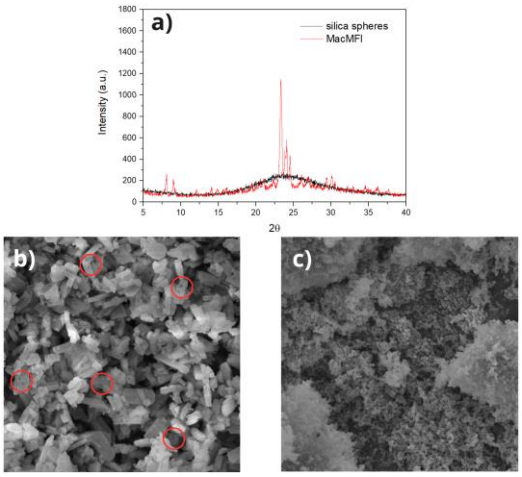


Figure 1: a) XRD of silica spheres and MacMFI. b) SEM of MacMFI. c) SEM of silica spheres.

Agradecimentos/Acknowledgments

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Green Synthesis of Potential Bioactive Limonene Derivatives via Catalytic Epoxidation and Cross-Metathesis

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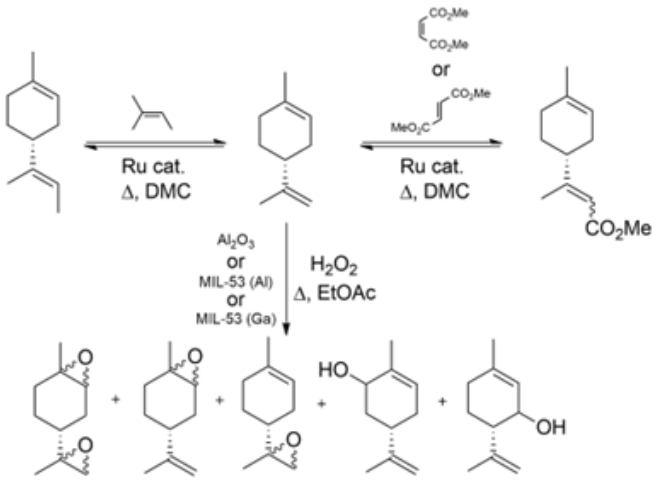
Palavras Chave:*Epoxidation,Metathesis,Catalysis,Organic Synthesis*

Highlights

Limonene derivatives were synthesized via epoxidation and cross-metathesis reactions with good conversion and will be tested for the first time against*T. cruzi*and*L. infantum.*

Resumo/Abstract

Chagas disease, caused by*Trypanosoma cruzi*, affects approximately six million people globally according to the WHO, with roughly one million cases reported in Brazil. Despite its documented adverse effects, benznidazole remains the primary therapeutic option for this neglected condition. Similarly, Leishmaniasis, caused by various*Leishmania*species, lacks a modern therapeutic arsenal, relying on outdated drugs. In this context, terpenes emerge as a strategic class of natural precursors. As the world's leading orange producer, Brazil offers an abundant supply of limonene, an ideal renewable platform for chemical synthesis. This project explores the structural diversification of limonene through two catalytic routes: cross-metathesis (CM) and epoxidation. Limonene derivatives were synthesized via CM using dimethyl maleate and 2-methylbut-2-ene as partners, catalyzed by ruthenium complexes under green conditions. Simultaneously, the library was expanded through epoxidation reactions using H_2O_2 over heterogeneous catalysts, including activated Al_2O_3 and Metal-Organic Frameworks (MOFs) developed by our group. Chromatographic analysis (GC-FID) showed CM conversions and yields ranging from 33–81%, respectively. The synthesized products, including the newly obtained epoxides, were isolated and characterized by GC-MS, ^1H and ^{13}C NMR. For the first time, these stable derivatives were evaluated for their biological activity against*T. cruzi*and*L.infantum*.



Green synthesis of limonene derivatives through cross-metathesis reactions and epoxidation with H2O2

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High-Entropy Oxides in Thermocatalysis: From Conventional Mixed Oxides to Entropy-Stabilized Materials

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Palavras Chave:*Keywords: Catalysis, Oxides, High Entropy Oxides, Exsolution,Catalysis,Oxides,High Entropy Oxides,exsolution*

Highlights

Transition metal oxides are widely used in catalysis, yet their evolution under reaction conditions and active sites remain underexplored. High-entropy oxides offer new opportunities and challenges.

Resumo/Abstract

Transition metal oxides are widely used in catalysis, yet their evolution under reaction conditions and the true nature of their active sites remain insufficiently understood. Their catalytic performance is increasingly recognized as a dynamic property, shaped by structural and chemical transformations that occur under working environments. This is particularly relevant for thermocatalytic reactions such as CO_2 hydrogenation and hydrodeoxygenation, where multiple reaction pathways depend sensitively on the nature of surface species.

In this context, advanced characterization techniques are essential to capture these transformations. In particular, near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) and in situ diffraction methods enable direct observation of changes in oxidation states, surface composition, and phase evolution under reaction conditions. These approaches provide unique insights into transient active states that cannot be accessed by conventional ex situ methods.

High-entropy oxides (HEOs) have recently emerged as a new class of materials, offering expanded compositional flexibility through the incorporation of multiple cations into a single lattice. This intrinsic disorder creates a responsive matrix capable of undergoing controlled restructuring processes, such as exsolution, in which metal species segregate from the bulk to form active surface nanoparticles.

The ability to monitor and tune these processes is key to understanding catalytic behavior. In particular, the composition of exsolved particles plays a central role in determining reactivity and selectivity. For CO_2 hydrogenation, the nature of the exposed metal governs pathways leading to CO, methanol, or CH_4, while in hydrodeoxygenation it influences C–O bond activation and competing reactions. These findings highlight the importance of coupling advanced in situ techniques with materials design strategies to establish robust structure–function relationships.

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Higher alcohols from syngas: in situ CO-DRIFTS insights on morphology effect of CeO2-supported Pt catalysts

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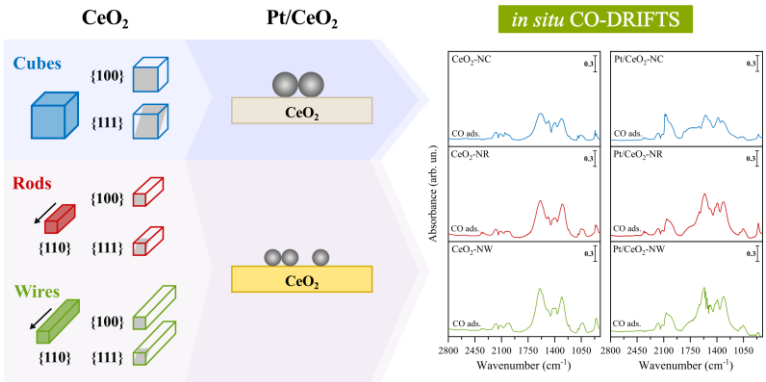
Palavras Chave:*CeO2 morphology,higher alcohols,DRIFTS,CO,surface interaction*

Highlights

A preliminary CO-DRIFTS study suggests that the morphology of CeO_2-supported Pt catalysts affects the formation and stability of key intermediate species involved in higher alcohol synthesis.

Resumo/Abstract

CeO_2-based catalysts are extensively investigated due to their ability to form a redox Ce^{3+}/Ce^{4+} pair, in which nanocrystals with well-controlled morphologies, different exposed facets, and oxygen vacancy content (Ov_ac) could enhance catalytic performance. In this work, rod-, wire-, and cube-shaped CeO_2 nanoparticle-supported Pt (1% wt.) catalysts were synthesized (named Pt/CeO_2- or CeO_2-NR, -NW, -NC, respectively). The physical-chemical properties of the catalysts were determined by XRD, Raman, XRF, N_2 physisorption, TPR-H_2 analyses, and HRTEM images. Surface chemical interactions of the catalysts were studied using*in situ*CO-DRIFTS to provide insights into higher alcohol (HA) synthesis from syngas. Temperature-resolved spectra were collected in He flow after pre-treatment and adsorption steps. The characterization confirmed the crystalline phase fluorite-type structure of CeO_2 and their morphologies. A higher concentration of reducible surface species indicates a larger proportion of crystal edges and corners, indicating a material with a smaller particle size, a lower crystallinity, and a higher surface area and concentration of Ov_ac, in accordance with the following sequence: NW ≈ NR → NC. The support's integrity was maintained after the addition of Pt, confirming the Pt-CeO_2 interactions and promoting H-spillover on the ceria surface. DRIFTS results revealed the morphology effect on the formation and stability of intermediate species across the temperature range, with varying proportions of adsorbed mono, bi, and polycarbonate species (v ≈ 1650-1050 cm^{-1}). Also, CO linear (terrace/corner sites) and bridging bonded to Pt particles were identified at 2100-1975 cm^{-1}. Particle size dependency is seen by intense narrow bands above 2060 cm^{-1} for NC (larger Pt particles) in comparison to NR/NW (smaller ones). Thus, CO non-dissociative adsorption on Pt and active sites of shaped ceria highlights the catalyst's versatility and potential for HA production from syngas.



In situ CO-DRIFTS analysis on Pt/CeO2 and CeO2 with different morphologies (cubes, rods and wires).

Agradecimentos/Acknowledgments

This work was supported by FINEP (project 01.23.0620.00). The authors would like to thank LABNANO/CBPF and Dr. M. Torquato for HRTEM.

Influência do teor de Cu nas propriedades do catalisador de Ni/H-ZSM-5 destinados a produção de H2 via decomposição catalítica do metano.

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Palavras Chave:*Zeólita ZSM-5,Catalisadores Bimetálicos de Ni-Cu,Decomposição Catalítica do Metano,Produção de Hidrogênio*

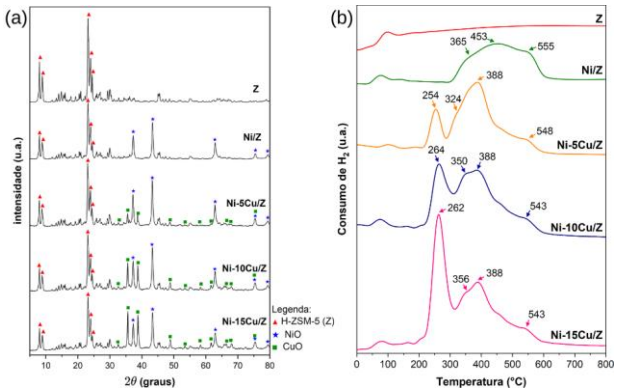
Highlights

Bimetallic Ni–Cu/H-ZSM-5 catalysts were successfully synthesized and characterized. The addition of Cu promoted the reduction of NiO to metallic Ni due to the spillover effect.

Resumo/Abstract

O agravamento da crise climática devido à utilização de combustíveis fósseis evidencia a necessidade de fontes energéticas sustentáveis. Nesse cenário, o hidrogênio se destaca como opção ecologicamente viável, e a decomposição catalítica do metano (DCM) surge como rota alternativa para sua produção, gerando simultaneamente hidrogênio e carbono sólido sem emissão direta de CO_2[1]. Este trabalho teve como objetivo sintetizar e caracterizar catalisadores bimetálicos de Ni-Cu suportados em zeólita H-ZSM-5 para futura aplicação na DCM. A síntese dos catalisadores foi realizada por impregnação incipiente sequencial (Ni seguido de Cu) sobre H-ZSM-5 (comercial), empregando-se um teor fixo de 20% de Ni e diferentes teores de Cu (5, 10 e 15%). As amostras sintetizadas foram caracterizadas por FTIR, DRX, FAAS, fisissorção de N_2 e TPR-H_2. A análise por FTIR confirmou a conversão eficiente de NH4 -ZSM-5 para a sua forma protônica da zeólita (HZSM-5, denominada Z) e todas as amostras apresentaram as bandas da estrutura da ZSM-5. A análise de DRX (Figura (a)) comprovou a presença das fases cristalinas da H-ZSM-5 em todas as amostras, do NiO nas amostras impregnadas, e a presença de CuO foi observada nas amostras contendo Cu como promotor, cuja a intensidade dos picos aumentou com a carga de Cu. Os resultados por FAAS mostraram teores experimentais de Ni próximos ao nominal (17,7-21,6%) e os teores de Cu foram superiores ao nominal. Observou-se que a adição dos metais não alterou a estrutura do suporte, exibindo isoterma do tipo I com ciclo de histerese H4. Os perfis de TPR-H_2 (Figura (b)) indicaram que todas as amostras foram totalmente reduzidas até 600 °C, e que a adição de cobre favoreceu a redução do óxido de níquel a níquel metálico. Os catalisadores bimetálicos Ni-Cu/H-ZSM-5 foram sintetizados e caracterizados com sucesso, apresentando propriedades físicas e químicas adequadas para a produção de hidrogênio via DCM.

[1]FAN, Zeyu et al.**J. Energy Chem.**, v. 58, p. 415-430, 2021.



Difratogramas de raios X (a) e perfis de TPR-H2 (b) das amostras sintetizadas.

Agradecimentos/Acknowledgments

Agradecemos ao PIBIC-UFBA, ao CNPq e aos grupos de pesquisa GCP, CATAM e GRPQQ.

Investigating the Metal–TiO2 Influence for Highly Selective Photocatalytic Oxidation of Methane to Methanol

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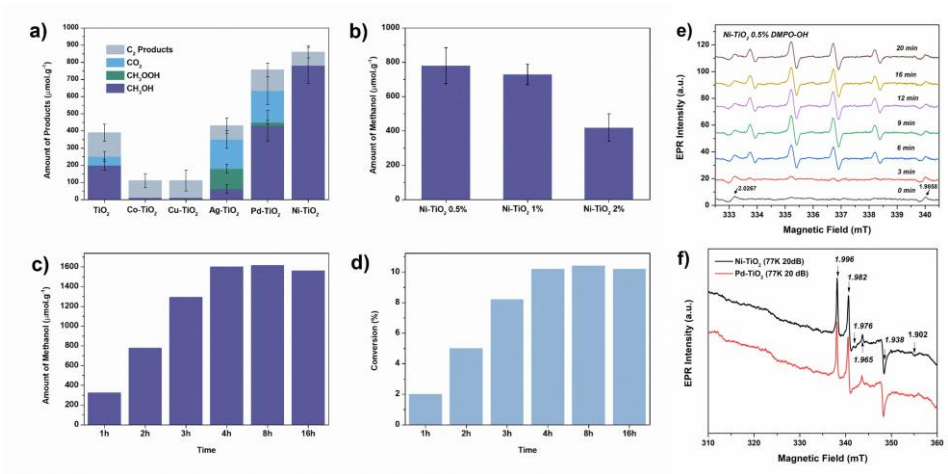
Palavras Chave:*Photocatalysis CH4 Oxidation, TiO2,Photocatalysis,Methane Oxidation,Titanium Dioxide*

Highlights

Methane photooxidation over metal–TiO_2 catalysts shows Ni-TiO_2 as highly selective, producing high methanol yields with minimal CO_2 via efficient •OH generation and improved charge trapping.

Resumo/Abstract

Methane conversion into value-added chemicals is a highly challenging yet desirable process. Photocatalysis offers a sustainable route for methane activation under mild conditions, avoiding the high temperatures and pressures required in conventional syngas-based processes. Titanium dioxide is the most widely used photocatalyst, but controlling methane oxidation on TiO_2 remains difficult due to overoxidation, which is strongly influenced by surface metal sites acting as heterojunctions. In this work, different metals were supported on TiO_2 and systematically evaluated for methane photooxidation. Among the catalysts tested, Ni-TiO_2 exhibited superior performance, achieving high methanol production (1600 μmol·g^{-1}) with minimal CO_2 formation using H_2O_2 as the oxidant. The enhanced activity and selectivity are attributed to the ability of nickel species to efficiently generate hydroxyl radicals, promote effective H_2O_2utilization, and induce charge-trapping sites such as Ti^{3+} centers and oxygen vacancies on TiO_2, which are crucial for C–H bond activation. This study sheds light on the role of catalyst structure in the proper control of CH_4 photoconversion.



a) Products; b) Methanol yield vs Ni; c) Methanol evolution; d) Methane conversion; e,f) EPR

Agradecimentos/Acknowledgments

The authors are thankful to CAPES, CNPq, Finep and FAPESP

Kinetic and Operando FTIR Investigation of Homogeneous Formic Acid Dehydrogenation Using CO_2 as a Spectroscopic Probe

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Palavras Chave:*formic acid dehydrogenation;,operando FTIR;,homogeneous catalysis;,ruthenium complexes;,reaction kinetics.*

Highlights

Operando FTIR using CO_2 vibrational modes provides real-time kinetic insight into homogeneous formic acid dehydrogenation catalyzed by ruthenium complexes.

Resumo/Abstract

The catalytic dehydrogenation of formic acid is a promising route for on-demand hydrogen generation under mild conditions. Since H_2 is infrared inactive, direct FTIR detection is not feasible. In contrast, CO_2, formed stoichiometrically during the reaction, presents infrared-active vibrational modes suitable for operando monitoring.

Carbon dioxide exhibits three fundamental vibrational modes: the IR-inactive symmetric stretch (v_1), the doubly degenerate bending mode (v_2), and the asymmetric stretch (v_3). Although the v_3 band at 2349 cm^{-1} is commonly used, it is strongly affected by atmospheric CO_2. In this work, the v_2 bending mode at 667 cm^{-1} was selected as a reliable spectroscopic probe, enabling operando monitoring of CO_2 formation without atmospheric interference.

Formic acid dehydrogenation was carried out under homogeneous catalytic conditions using the organometallic ruthenium complex [RuCl(*p*-cymene)(N–N)](PF_6), where N–N = N^1,N^2-bis(2,6-dimethylphenyl)ethane-1,2-diimine, developed in our laboratory. Operando FTIR measurements were performed using a Shimadzu IRTracer-100 spectrometer equipped with a cryogenically cooled MCT detector, coupled to a gas cell (98 mL, KRS-5 windows). The system was purged with argon to suppress residual CO_2 under flow conditions.

Kinetic profiles were obtained by integrating the v_2 band area as a function of time and analyzed using a sigmoidal growth model ($X_{mo}d_{el}$), allowing the extraction of observed rate constants (k_ob_s). Temperature-dependent kinetic data yielded apparent activation energies of 86.7 k*J*mol^{-1} (Arrhenius analysis), while Eyring analysis provided activation parameters of $\Delta H‡$ = 83.8 kJ mol^{-1} and $\Delta S‡$ = −71.1 J mol^{-1} K^{-1}, consistent with a homogeneous catalytic mechanism. Hydrogen purity was evaluated by GC-TCD.

These results demonstrate that real-time FTIR spectroscopy is a powerful operando tool for quantitative kinetic studies of homogeneous formic acid dehydrogenation.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPEMIG, CNPq, and CAPES, as well as the institutional support of the Federal University of Uberlândia (UFU).

Kinetic/thermodynamic study of the production of biodiesel using a porous carbon-supported catalyst obtained from ornamental stone tailings

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Palavras Chave:*Biodiesel,Heterogeneous catalysis,Reaction kinetics,Ornamental stone tailings,Coconut shell activated carbon*

Highlights

- Innovative activated carbon / stone tailings catalyst yielded 96% biodiesel conversion.

- Transesterification reaction was successfully described using a pseudo first-order kinetic model.

Resumo/Abstract

Dependence on fossil fuels has intensified environmental problems, particularly greenhouse gases (such as CO_2). In this context, the rise of biodiesel as a sustainable alternative is noteworthy. This study investigated the kinetic and thermodynamic aspects of the transesterification of soybean oil with methanol, catalyzed by an innovative heterogeneous carbon-based catalyst derived from ornamental stone tailings. The catalyst was prepared by impregnation, activated carbon (obtained from coconut shells) and ornamental stone tailings were initially added to a 3.75 mol/L NaOH solution. Subsequently, the material was dried and subjected to heat treatment at 800 °C for 1 h. After heat treatment, the catalysts presented 21.1, 10.2, and 53.3% m/m of CaO, MgO, and Na_2CO_3, respectively. The phases are dispersed in the carbon matrix. For the thermokinetic study, the reactions of biodiesel production were conducted at 30, 45, and 60 °C. Aliquots were collected at 60, 120, and 180 min, and the catalyst was removed using 0.45 µm membranes. Biodiesel conversion was quantified by solution ^{1}H NMR, reaching a maximum of 96%. The determined rate constants (k) were 8.6×10^{-4}, 6.7×10^{-4}, and 2.4×10^{-2} min^{-1} for 30, 45, and 60 °C, respectively. A pseudo-first-order model successfully described the reaction, with relatively high values of the determination coefficients R^2 (0.95–0.99). The E_a was 90.1 kJ/mol, showing a high thermal dependence. The values of ΔH = +88.2 kJ/mol, ΔS = -17.7 J/(mol·K), and ΔG = +94.1 kJ/mol indicate an endothermic, nonspontaneous process. The negative ΔS suggests a more ordered activated complex, characteristic of associative mechanisms in the rate-determining step. Furthermore, the proposed route effectively dispersed the active phases, preventing the leaching of Ca and Mg and ensuring compliance with EN-14214 standards.

Agradecimentos/Acknowledgments

FAPES, CAPES, CNPq, CETEM, UFES, LABPETRO, LUCCAR.

Layered double hydroxides of Cu/Al as efficient catalysts in the production of carbohydrate-derived fatty esters

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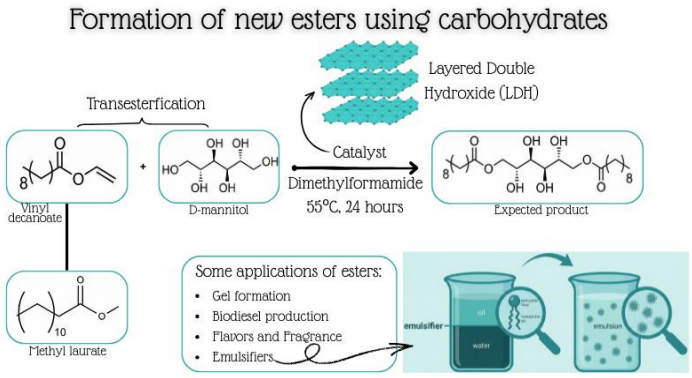
Palavras Chave:*Transesterification,LDH,Vinyl decanoate,D-mannitol,Methyl laurate*

Highlights

Catalytic transesterification reaction between fatty acid esters and D-mannitol showed high conversion and selectivity for one diester, with superior performance of the Cu/Al LDH.

Resumo/Abstract

Catalytic transesterification is key for synthesizing new esters. Among these, carbohydrate-functionalized fatty esters are vital as biofuels, biolubricants, and green emulsifiers. This work evaluates producing amphiphilic esters via transesterification of medium-chain fatty esters (C10–C12) with D-mannitol. The assays were performed using vinyl decanoate (or methyl laurate) and D-mannitol under mild reflux (55°C) for 24 hours, in the presence of a Cu/Al layered double hydroxide (LDH) (Neves et al., 2017). In addition, commercial basic and amphoteric catalysts were tested as catalytic controls (K2CO3, MgCO3, CaCO3, (NH4)H2PO4, or NaH2PO4). Under these conditions, the use of Cu/Al LDH led to conversions of the precursor esters in the range of 90–95%, with selectivity towards a disubstituted product (di-O-decanoyl mannitol and di-O-lauryl mannitol) of approximately 80%. In the case of carbonates, a decrease in catalytic selectivity (approximately 45%) was observed, while the use of dihydrogen phosphates led to lower conversions, with major selectivity to the monosubstituted product. In all cases, the use of DMF allowed catalytic conversions superior to acetonitrile. ^{1}H NMR spectra suggested the formation of the transesterification product through the emergence of singlets between 2.2 and 2.3 ppm. According to the literature, Cu (II) ions are very effective in the esterifications/ transesterifications (Hossain et al., 2019).This fact reinforces the superiority compared to Mg/Al LDH — both prepared by co-precipitation from metal salts solution using constant pH approach and intercalated with carbonate anions (CO_3^{2-}) (Neves, VA et al. J. Therm. Anal. Calorim. 2017, 130, 689.) —, whose activity was approximately 25% lower under the evaluated conditions. Finally, the layered system proved to be active (conversions above 90%), even after three reuse cycles. Studies are underway for the determination of the structure along with the catalytic evaluation of other carbohydrates



Formation of new esters using carbohydrates

Agradecimentos/Acknowledgments

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Mechanistic study of the synthesis of MoV2O8 mixed oxides via mechanochemistry

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Palavras Chave:*Mechanochemistry,Synthesis,MoV2O8 Mechanism,MoV2O8,Mechanism*

Highlights

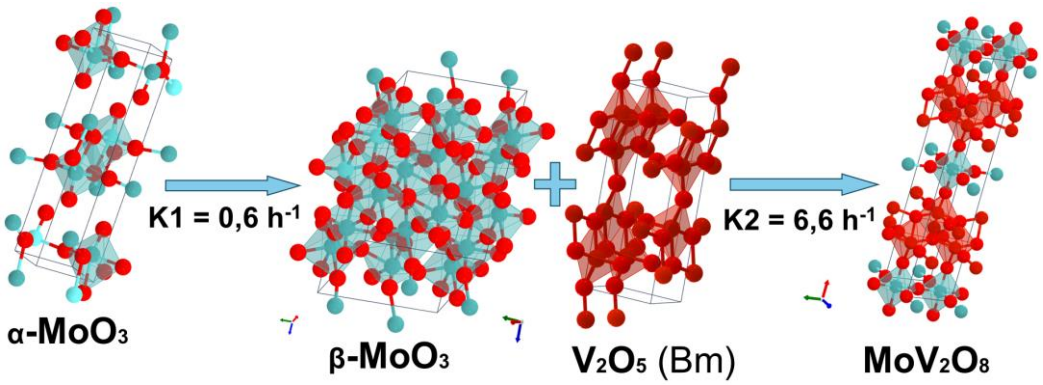
The synthesis achieves maximum MoV2O8 percentage in 6 hours.

During milling, α-MoO3 transforms into β-MoO3.

The presence of beta-molybdenum accelerates the mixed oxide formation reaction.

Resumo/Abstract

Molybdenum (Mo) and vanadium (V) metal oxides are of great importance in the field of catalysis due to their ability to generate reactive oxygen species, being widely used in catalytic oxidation reactions. The synergy present in the mixed oxide leads to characteristics that surpass those of their individual oxides, resulting in greater efficiency in catalysis. Until now, the synthesis of this compound was limited to mainly hydrothermal and solvothermal methods, which demand high temperatures and long reaction times. Mechanochemistry emerges as a sustainable and efficient alternative, utilizing only mechanical energy for the reaction, thus reducing synthesis temperature and time without the use of solvents. In this work, systematic syntheses of the MoV2O8 mixed oxide were carried out via the mechanochemical route starting from MoO3 and V2O5, characterizing the synthesis products by X-ray diffraction (XRD) and quantified by the Rietveld refinement method, in addition to N2 physisorption and transmission electron microscopy (TEM). The results show that maximum conversion of the mixed oxide (95.65%) was achieved in 6 hours. The investigation of the mixed oxide formation mechanism revealed that orthorhombic MoO3 (α-MoO3) changes its crystal structure to monoclinic (β-MoO3) during milling, and kinetic calculations show that once transformed into β-MoO3, the reaction occurs much more rapidly. To confirm this information, the reaction was tested starting directly from β-MoO3 synthesized by traditional chemical methods and mechanochemically synthesized. It was confirmed that the addition of monoclinic molybdenum accelerates the formation of the mixed oxide (95.22% of MoV2O8 was achieved in 3 hours of milling using chemically synthesized β-MoO3 and 95.22% in 2 hours using mechanochemically synthesized β-MoO3), suggesting that the transformation of α-MoO3 to β-MoO3 is a determining step in the kinetics of MoV2O8 formation.



Representation of the mixed oxide formation and its intermediates with rate constants

Agradecimentos/Acknowledgments

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Metal-Beta zeolites for poly(lactic acid) alcoholysis

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Palavras Chave:*heterogeneous catalysis,polymer,chemical recycling,green chemistry*

Highlights

In this work, we use multiple well-characterized metal-zeolite catalysts, such as Al-Beta, Sn-Beta, Hf-Beta, and Zr-Beta, for the alcoholysis of polylactic acid.

Resumo/Abstract

Poly(lactic acid) (PLA) is a biopolymer obtained through the polymerization of lactide, a cyclic dimer derived from lactic acid, which is produced by the fermentation of sugars from sugarcane or corn. According to European Bioplastics, PLA was the most produced bioplastic in 2023, accounting for 31.0% of global production.

The conversion of PLA via alcoholysis constitutes a chemical recycling route for the production of alkyl lactates, which are platform chemicals for a wide range of products or can be directly used as green solvents due to their good biodegradability and low toxicity. Chemical depolymerization is energetically more favorable than the production of virgin polymer, since the latter involves a costly fermentation route.

Zeolites are crystalline microporous materials based on TO_4 tetrahedra (T = Si, Al, etc.), whose properties can be tuned through isomorphic substitutions. The incorporation of Al generates Brønsted acid sites, whereas metals such as Sn, Zr, and Hf can introduce Lewis acidity. In this context, Beta-type zeolites containing different heteroatoms can act as acid catalysts in the alcoholysis of PLA, promoting the nucleophilic attack of the alcohol on the carbonyl carbon of the polymer. Al-Beta, Sn-Beta, Hf-Beta, and Zr-Beta zeolites were prepared by hydrothermal synthesis (fluoride medium) and characterized by XRD, N_2 adsorption, ICP, TGA, DRS, SEM, and solid-state NMR (^{29}Si and ^{27}Al). The characterizations indicated the formation of submicrometric Beta zeolite particles with Si/M ratios close to 30 for Al-Beta and 100 for the other M-Beta samples. All solids exhibited mesoporosity with a low degree of defects, except for the Sn-Beta sample. DRS and ^{27}Al NMR analyses indicated that the heteroatoms were predominantly incorporated into the zeolitic framework. Alcoholysis reactions are currently underway at the time of writing.



SEM images of Al-Beta, Sn-Beta, Zr-Beta, and Hf-Beta (from left to right)

Agradecimentos/Acknowledgments

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MgO support catalysts prepared by sol-gel method for CO2 methanation

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Palavras Chave:*CO2 Methanation, Heterogeneous Catalysis, Ni/MgO Catalysts, Sol-Gel Synthesis*

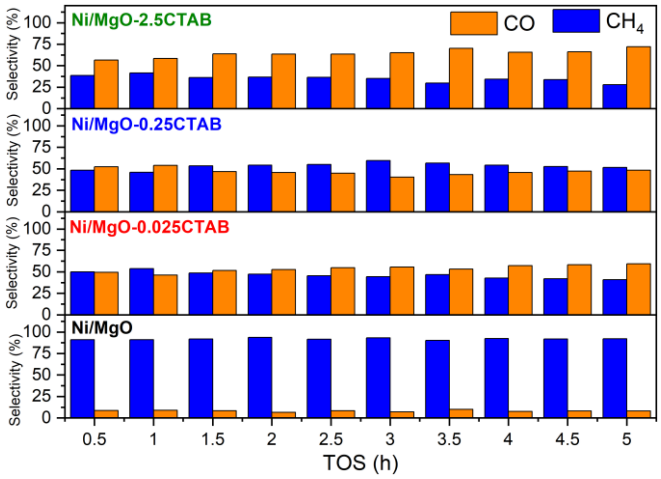
Highlights

Synthesis by the sol-gel method using CTAB surfactant, changes in texturial properties.

Ni/MgO catalysts with high oxygen vacancy values aplication on CO_2 methanation.

Resumo/Abstract

In this work, it was possible to study the effects of sol-gel synthesis and how it affects the catalyst structure, making it possible to control effects such as roughness, surface area size and vacancies. Vacancies play an important role in CO_2 reduction reactions, mainly by facilitating the adsorption of CO_2 in the catalyst structure. In addition, nickel, the active phase used in this work, can replace Mg in the structure, thus hindering processes that deactivate the catalyst, such as sintering. The Ni/MgO sample was a sample that underwent the synthesis process, but without the CTAB surfactant. The use of sol-gel synthesis alone was effective in structurally modifying MgO, where it presented an oxygen occupancy of 0.94. However, the introduction of CTAB increased the volume of vacancies, where it increased to occupancy of 0.82, in the sample with the lowest CTAB concentration. After undergoing the nickel impregnation process, modified vacancy values were obtained, where the most significant was the Ni/MgO-0.025CTAB sample, which went from 0.82 oxygen occupancy to 1.00, and it was possible to observe that the previously present vacancies were filled. The possibility of nickel having been deposited in the interstice of the MgO structure is related to its catalytic activity.



Selectivity of Ni/MgO catalysts during the reaction

Agradecimentos/Acknowledgments

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Microwave synthesis of iron oxide/carbonaceous material composites for use in photocatalysis and adsorption

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Palavras Chave:*Iron oxide nanoparticles,Sugarcane bagasse,Wastewater treatment process,Methylene blue,Iron oxide nanoparticles; Sugarcane bagasse; Wastewater treatment process; Methylene blue.*

Highlights

Microwaves were used in the synthesis of new iron oxide/carbonaceous material composites with good photocatalytic and adsorption performance. The leaching of iron oxide during adsorption was reduced.

Resumo/Abstract

Iron oxide (IO) nanoparticles are widely applied in wastewater treatment processes, such as adsorption and heterogeneous photocatalysis, due to their properties, which can be improved by combining with carbonaceous materials (CM) derived from biomass, forming composites. Microwave-mediated synthesis stands out as a fast, efficient, and sustainable method for obtaining these materials. This work aimed to obtain new OF/MC composites from a mixture of iron oxide nanoparticles and sugarcane bagasse (BC), using microwave-assisted heating, for application in adsorption and heterogeneous photocatalysis processes, employing methylene blue (MB) as a model contaminant. Iron oxide nanoparticles (OFM) were obtained by heating iron(III) nitrate in a microwave muffle (200 °C, 10 min). Next, the nanoparticles were mixed with sugarcane bagasse and subjected to heat treatment in a microwave muffle at 200 °C (OFM-BC-200) and 300 °C (OFM-BC-300) for 10 min. The materials were characterized using different techniques. Photocatalytic tests were conducted as shown in Figure 1, while adsorption experiments were performed using 100 mg of the composites and MB solutions with concentrations between 1.0 and 6.0 mg L^{-1} (stirring, 1 h). Pure iron oxide exhibited a band gap energy of 2.01 eV, promoting 98% discoloration of the MB through heterogeneous photocatalysis; however, it was not possible to carry out adsorption tests due to the high leaching of iron. The OFM-BC-200 and OFM-BC-300 composites exhibited a hematite phase, a band gap around 2.00 eV, and high efficiency in MB decolorization by adsorption and photocatalysis. It is concluded that the synthesis employed was efficient in obtaining new composites with good performance in photocatalysis and adsorption, reducing iron leaching, they are promising for environmental applications, with the OFM-BC-200 material standing out.

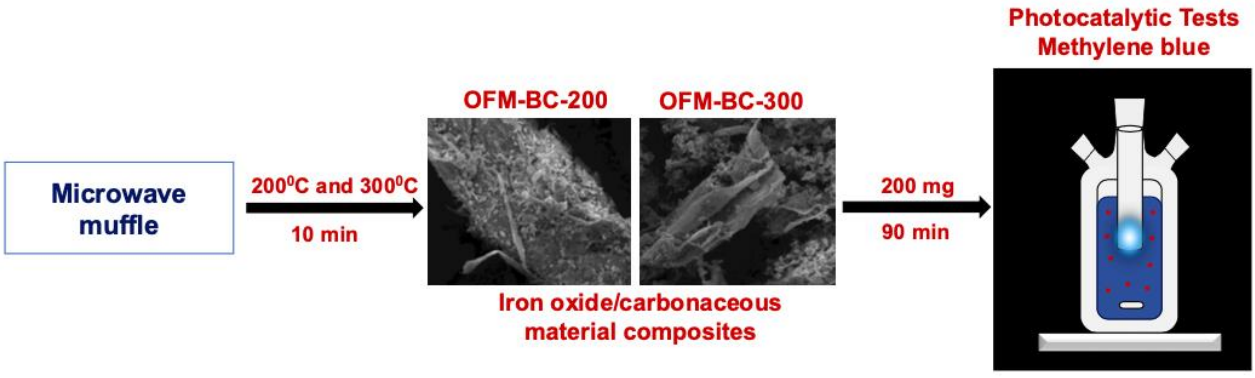


Figure 1. Experimental procedure for synthesizing composites and photocatalytic tests.

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MOF-derived synthesis of metal oxides with supported cesium.

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Palavras Chave:*MOF-derived, cesium incorporation, thermal treatment.*

Highlights

MOF-derived ZrO_2 and Co_3O_4 were obtained from UiO-66, UiO-67 and ZIF-67 and modified with cesium by incipient wetness impregnation.

Resumo/Abstract

Metal–Organic Frameworks (MOFs) constitute a class of porous materials formed through the interaction between metal ions or clusters and organic ligands. The interest in these materials has grown rapidly due to their properties, such as high crystallinity, microporosity, high surface area, low density, and the possibility of pore functionalization. This set of characteristics makes MOFs excellent materials for applications in several research areas, including gas storage and separation and heterogeneous catalysis. In addition, many studies have investigated MOFs as precursor materials, playing a role as templates for the construction of micro- and nanostructured materials, such as porous carbons and metal oxides, through high-temperature thermal treatment. In these derived materials, chemical modification is still possible through the incorporation of alkaline species as a strategy to tune the chemical reactivity of these structures. The present work presents the synthesis and characterization of ZrO_2 and Co_3O_4 derived from the UiO-66, UiO-67, and ZIF-67 MOFs, containing supported cesium-based species via the incipient wetness impregnation method. Synchrotron X-ray diffraction patterns indicated the conversion of the precursor MOFs into derived metal oxides, evidenced by the absence of reflections characteristic of the original structures and by the presence of a semicrystalline profile, with crystalline peaks superimposed on an amorphous halo. Scanning electron microscopy images reveal the formation of micrometric aggregates with irregular morphology, with textural differences associated with the thermal treatment and the precursor used. EDS analyses confirmed the presence of the constituent elements of each oxide, as well as the incorporation of cesium in all samples, indicating its distribution throughout the derived materials. Subsequently, these materials will be evaluated as catalysts in the transesterification reaction of glycerol.

Agradecimentos/Acknowledgments

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Molten Salt–Driven Breakdown of Cutin: A Shortcut to High-Value Bio-Based Monomers

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Palavras Chave:*Cutin,Biomass,Molten Salt,ácido 10,16-diidroxi-hexadecanoico*

Highlights

Cutin was depolymerized in one-pot using hydrated molten salts and zeolite, enabling the efficient conversion of 10,16-DHHA for integration into biorefineries and valorization of agro-industrial waste

Resumo/Abstract

Cutin, a natural biopolyester, comprises the outer protective layer of plants, known as the cuticle, acting as a barrier against water loss, microorganism attacks, and physical damage. Structurally, it is formed by long-chain fatty acids, predominantly C16 and C18, with C16 dihydroxylated fatty acids being the most abundant, accounting for over 60% of its weight. This biopolymer is widely found in agricultural residues, such as tomato and apple peels, and can be easily recovered for application in industrial processes. In this work, the depolymerization of cutin present in tomato peel was conducted using molten salt hydrate systems ($LiBr{\cdot}3H_2O$ and $ZnCl_2{\cdot}3H_2O$, designated LiP and ZnP, respectively) combined with HZSM-5 zeolite as an acid catalyst, aiming at the efficient valorization of this residue in a single step. The treatments were performed under mild conditions (90 °C, 2 h, 600 rpm). Under these conditions, LiP and ZnP exhibited high conversions to soluble products (44.2 ± 3.2% and 63.4 ± 5.2%, respectively). The addition of the HZSM-5 catalyst resulted in the complete hydrolysis of the biomass, suggesting that the high density of Brønsted acid sites in the zeolite's aqueous phase (813 $\mu molg^{-1}$) and its high specific surface area (446 m^2g^{-1}) contributed to the one-pot depolymerization of cutin. The major product obtained was 10,16-dihydroxyhexadecanoic acid (10,16-DHHA), a versatile monomer applicable in the synthesis of biopolymers, surfactants, organic synthesis intermediates, and biofuels. Overall, the catalytic approach employing molten salt hydrates demonstrates significant potential for integration into biorefineries, enabling the production of dihydroxylated acids with high yield and adding value to these agro-industrial residues.



Overview of the processes involved in cutin depolymerization.

Agradecimentos/Acknowledgments

The authors acknowledge CNPq (Process No. 446696/2024-2) for financial support and Grupo de Catálise e Valorização da Biomassa/GCVB at Federal Fluminense University for supporting the development of the research.

Ni/CaO and Ni/CaO@SiO2 catalysts applied to the dry reforming of methane.

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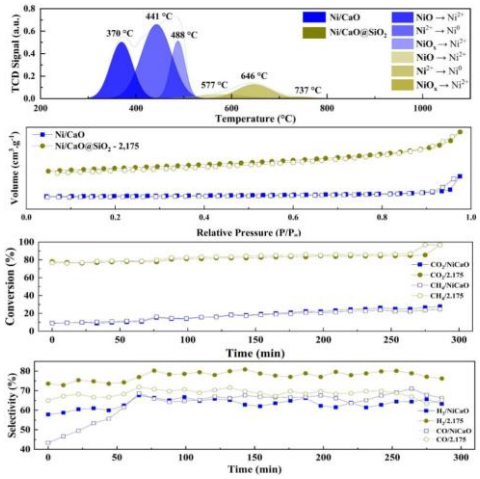
Palavras Chave:*CO2 Capture,Dry Reforming of Methane,Heterogeneous Catalysis,Mesoporous SiO2,Dual-Function Materials. ,CO2 capture,Dual-Function Materials*

Highlights

Aiming at high-temperature stability and sintering mitigation in catalytic conversion, the Ni/CaO@SiO_2 catalyst was prepared for CO_2 conversion into syngas by the dry reforming of CH_4.

Resumo/Abstract

Addressing the energy challenge associated with high greenhouse gas emissions, mainly CO_2 and CH_4, the synthesis of Ni/CaO and Ni/CaO@SiO_2 materials was proposed as catalysts for CO_2 conversion through dry reforming of methane, exploring the correlation between Ni metallic sites, responsible for CH_4 activation, and the basicity of CaO, which favors CO_2 adsorption and activation. Accordingly, using the Stöber method, a core@shell architecture was targeted for the Ni/CaO@SiO_2 catalyst, resulting in a sample with a specific surface area of approximately 178 $m^2.g^{-1}$, a marked increase in pore volume, and pore diameters within the mesoporous range, thereby promoting efficient diffusion of reactants and products to the active sites. As expected, the SiO_2 layer acted as a physical barrier against sintering, stabilizing the metallic particles, modulating Ni reducibility, and contributing to the mitigation of carbon deposition, thus preserving metal dispersion under severe operating conditions. Morphological and textural analyses (TGA, TPR, N_2 physisorption, XRD, SEM, and TEM) indicated that TEOS-derived coating leads to homogeneous encapsulation, stronger metal–support interaction, and improved morphological control compared to the uncoated Ni/CaO. Furthermore, in fixed-bed catalytic tests for DRM, Ni/CaO@SiO_2 exhibited CH_4 and CO_2 conversions above 80%, an H_2/CO ratio close to 1, and selectivity higher than 90% for H_2 and CO, significantly outperforming the activity and stability of Ni/CaO, which, despite its good initial performance, suffers from nanoparticle sintering and filamentous coke deposition, leading to rapid deactivation at the high temperatures typical of DRM, thereby making the proposed system a promising candidate for high-temperature CCUS technologies.



TPR profiles, N2 adsorption isotherms, CO2/CH4 conversion, and H2/CO selectivities in DRM

One-pot synthesis of methyl oleate from canola oil catalyzed by Eversa Transform 2.0

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Palavras Chave:*hydrolysis,fatty acid,esterification,methyl ester.*

Highlights

Canola oil hydrolysis yielded 93% of free fatty acids.

84% of fatty acid methyl esters was achieved after esterification.

Methyl oleate was successfully synthesized via a batch cascade reaction.

Resumo/Abstract

The development of green chemistry has increased the use of renewable raw materials as alternatives to petrochemicals[1]. Fatty acid methyl esters (FAMEs) are monoalkyl esters synthesized from various renewable feedstocks. Among them, methyl oleate is highlighted for its wide application in chemical engineering, pharmaceuticals, agriculture, and other industrial fields [2]. The objective of this work was to evaluate the potential of lipase Eversa® Transform 2.0 to synthesize methyl oleate in a one-pot reaction. Canola oil was used as a raw material due to its high oleic acid content (58-65%) and its lower price compared to other oils also rich in oleic acid [3]. To optimize the hydrolysis reaction, a central composite rotatable design was prepared with three independent variables: buffer molarity (100 – 200 mM), lipase concentration (1 – 3 % w/w), and temperature (50 – 70°C). The hydrolyzed fractions, as well as FAME formation, were analyzed by gas chromatography. After the optimization process, the optimal conditions for the hydrolysis of canola oil were 170 mM buffer, 2.3% w/w lipase, and 72.8 °C, resulting in a total acid content of 93.3 ± 1.19% within 4 hours. Esterification proceeded directly following hydrolysis in a one-pot process, eliminating the need to isolate free fatty acids, remove water, or add supplemental lipase. To prevent enzymatic inactivation, methanol was introduced in six steps with an oil-to-methanol molar ratio of 1:4.9 at 40 °C for 6 hours. The reaction yielded an 84.0 ± 2.1% conversion to methyl esters, with methyl oleate accounting for 61.8 ± 2.6% of the total. These results validate enzymatic cascade synthesis as a promising route for the large-scale production of methyl oleate. The integration of reactions maximizes productivity and reduces operational costs.

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One-step fractionation and upgrading of coconut fiber by molten salt hydrate and acid catalysis

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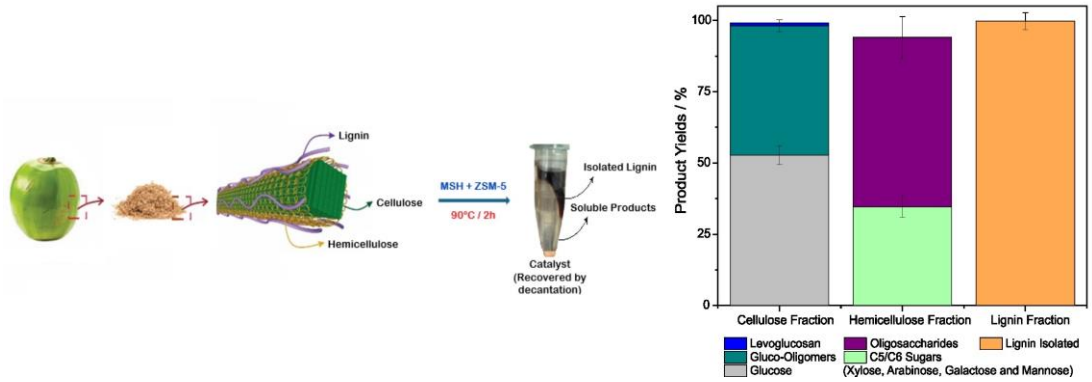
Palavras Chave:*Coconut fiber,Zeolite catalysis,Molten salt hydrate,Biomass fractionation*

Highlights

Biomass valorization enabled by a LiBr·3H_2O-Zeolite catalytic system. Brønsted acidity of HZSM-5 promotes carbohydrates depolymerization. High sugar yields and near-quantitative lignin recovery.

Resumo/Abstract

Lignocellulosic biomass from agro-industrial residues represents an abundant and underexploited source of renewable carbon. Among these residues, coconut stands out due to its high lignin content and large availability in Brazil[1]. In this work, coconut fiber (0.05 g) was selectively fractionated using a molten salt hydrate system (LiBr·3H_2O, 2.5 g) combined with HZSM-5 zeolite (Si/Al = 11.5, 0.05g) as an acid catalyst, aiming at the efficient valorization of cellulose, hemicellulose, and lignin in a single step. The treatment was conducted under mild conditions (90 °C, 2 h and 600 rpm), leading to effective disassembly of the lignocellulosic matrix and catalyst recovery. The catalytic performance is directly associated with the textural and acidic properties of HZSM-5, which exhibits a micro-mesoporous structure (MFI type), high specific surface area (418 $m^2\ g^{-1}$), and a high density of Brønsted acid sites in aqueous phase (600 $\mu mol\ g^{-1}$). Under these conditions, the cellulose fraction showed high conversion to soluble products (Fig. 1), yielding 52.7 ± 3.2% glucose and 45.4 ± 2.1% gluco-oligomers, with only minor formation of levoglucosan (1.0 ± 0.1%). For the hemicellulose fraction, the process favored oligomer formation, producing 59.4 ± 7.4% oligosaccharides and 34.6 ± 3.6% C5/C6 sugars, including xylose, mannose, galactose, and arabinose. Remarkably, the solid residue recovered after treatment consisted almost exclusively of lignin, with an isolation yield of 99.8 ± 2.9%, evidencing the high selectivity of the molten salt hydrate–catalyst system toward carbohydrate solubilization while preserving lignin integrity. Overall, this catalytic molten salt hydrate approach demonstrates strong potential for integrated biorefinery applications, enabling high-yield sugar production, avoiding degradation products and a near-quantitative lignin recovery from coconut fiber in a one-step process.
[1] Rambo, M.*et al.Talana.*144, 696-703 (2015)



Products distribution after coconut fiber processing in LiBr·3H2O/ZSM-5 at 90 °C

Agradecimentos/Acknowledgments

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Optimizing Ruthenium-Catalyzed Cross-Metathesis: Methodological Development from Model Alkenes to Complex Bioactive Frameworks

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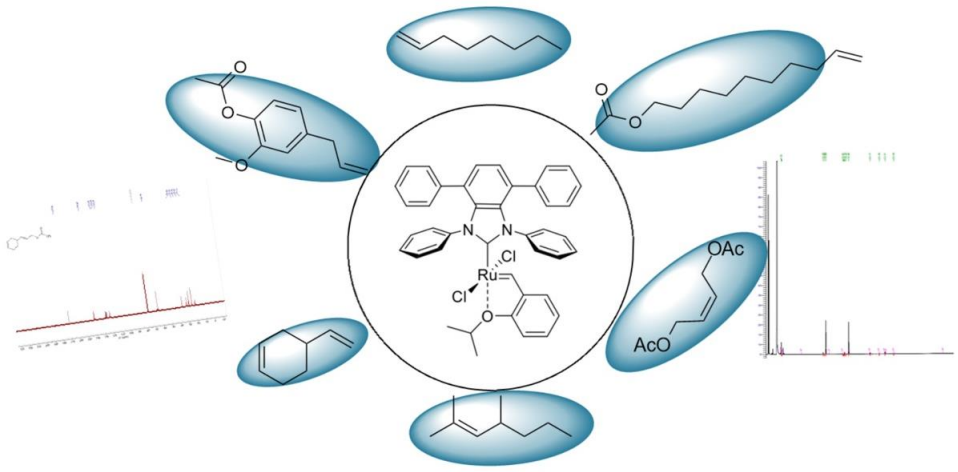
Palavras Chave:*Ruthenium, Grela´s Catalysis, Cross-Metathesis, Organic Synthesis,Ruthenium, Catalysis, Cross-Metathesis, Organic Synthesis.*

Highlights

A robust cross-metathesis framework using ruthenium catalysts achieved up to 72% isolated yield and 96% selectivity, validating a platform for diversifying complex bioactive molecules.

Resumo/Abstract

The efficiency of catalytic olefin metathesis is fundamentally tied to the compatibility between catalyst architecture and substrate reactivity. This research focused on establishing a robust synthetic and analytical framework for cross-metathesis (CM), aimed at optimizing protocols for future applications on structurally sophisticated and sensitive bioactive molecules. The study utilized model alkenes, such as eugenol acetate and 4-vinyl-1-cyclohexene, to evaluate the performance of specialized ruthenium-based catalystReactions were conducted under mild conditions using a catalyst developed and synthesized by Grela's group, with precise catalyst additions followed by strategic quenching and isolation procedures. A primary objective was to evaluate the influence of nitro-substituted ruthenium complexes on reaction selectivity. The experimental groundwork addressed critical challenges in CM, including catalyst deactivation and the purification of functionalized derivatives, ensuring a reliable pathway for producing high-purity unsaturated compounds. The investigation culminated in a highly successful CM between 4-vinyl-1-cyclohexene and cis-1,4-diacetoxy-2-butene. This system provided the target products with an outstanding 72% isolated yield and 96% selectivity, as confirmed by GC-FID and NMR analysis. These results represent a significant advancement over earlier attempts with eugenol acetate, where purification challenges limited isolated yields to 29%. This rigorous protocol establishes a proven, effective synthesis and purification framework, setting the stage for the diversification and biological evaluation of more complex and sensitive chemical structures.



Study on the performance of new ruthenium-based catalyst for Cross-Metathesis reactions using model

Agradecimentos/Acknowledgments

FAPESP, CAPES, CNPq, UFABC, University of Warsaw

Oxygen Evolution Mediated by Ionic Carbon Nitrides Functionalized with Ruthenium Complex

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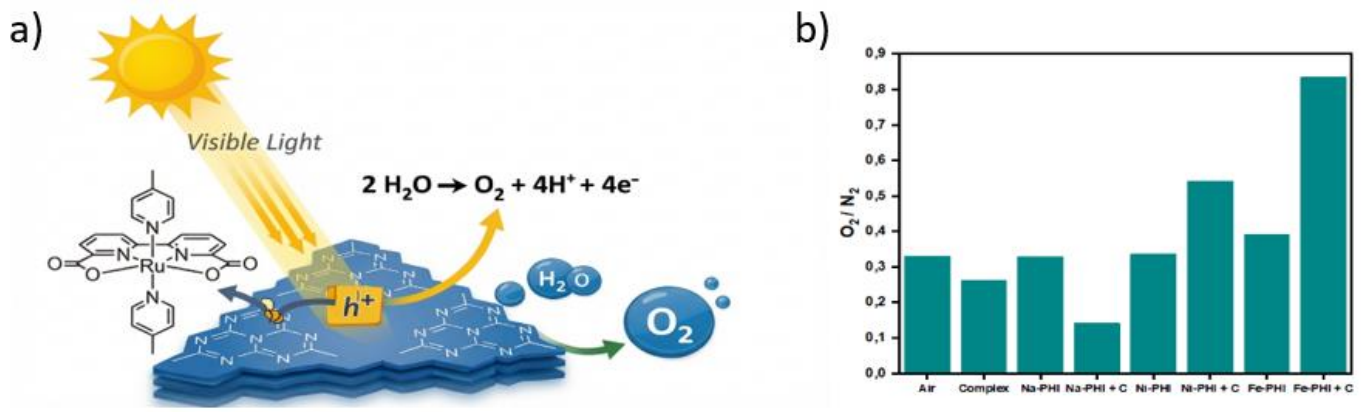
Palavras Chave:*Photocatalysis, Water oxidation, Oxygen evolution, Carbon Nitrides, Ruthenium complexes.,Photocatalysis, Water oxidation, Oxygen evolution, Carbon Nitrides, Ruthenium complexes.*

Highlights

PHI materials functionalized with ruthenium complexes for visible-light-driven water oxidation, Efficient and stable oxygen evolution under mild aqueous conditions.

Resumo/Abstract

Water oxidation is a key process in artificial photosynthesis and solar energy conversion, yet it remains limited by sluggish kinetics and inefficient charge management. Photocatalytic systems based on carbon nitrides offer a promising route to drive the oxygen evolution reaction under mild conditions using visible light. In particular, ionic carbon nitrides such as poly(heptazine imide) (PHI) provide well-defined structures, improved charge transport, and the ability to interact with metal species. In this work, PHI materials combined with transition metal centers and ruthenium complexes were investigated for visible-light-driven water oxidation. The photocatalytic activity was evaluated by monitoring oxygen evolution, quantified as the O_2/N_2 ratio. Among the systems studied, the Fe–PHI material combined with a ruthenium complex (C) exhibited the highest activity, reaching an O_2/N_2 ratio of 0.8 under the investigated conditions. Structural characterization by infrared spectroscopy revealed noticeable changes in the PHI-based materials after photocatalytic operation, indicating modifications in the local chemical environment induced by the reaction. These results highlight the influence of metal centers and molecular complexes on the photocatalytic performance of ionic carbon nitrides and provide insights into the design of efficient systems for oxygen evolution reactions.



1.a) Scheme of the visible-light-driven photocatalytic water oxidation reaction. b) O2/N2 ratio

Agradecimentos/Acknowledgments

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Pequi peel (Caryocar brasiliense) impregnated with molybdenum as a heterogeneous catalyst in biodiesel production.

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Palavras Chave:*Casca de pequi,biorresíduos,catalisador heterogêneo,biodiesel.,Pequi peel*

Highlights

Catalyst based on pequi peel impregnated with molybdenum.

The material achieved 99.5% yield of methyl esters.

It showed good stability and reusability for up to 10 cycles.

Resumo/Abstract

Biodiesel has established itself as a renewable and sustainable alternative to fossil fuels, driving research aimed at optimizing its production process. In this scenario, the development of catalysts derived from biomass waste emerges as a promising approach for more sustainable production. This work aimed to synthesize a heterogeneous catalyst from pequi peel impregnated with $(NH_4)6Mo_7O_{24}\cdot 4H_2O$. The resulting solid was dried at 105 °C for 4 h and characterized by FTIR, TGA, SEM-EDS, and surface area by the BET method. FTIR analysis of the biomass revealed characteristic bands of cellulose, hemicellulose, and lignin. After impregnation, the appearance of bands in the 1000–500 cm^{-1} region, attributed to Mo–O stretching vibrations, indicates the anchoring of the metal on the biomass surface. Thermogravimetric analysis identified three stages of degradation: moisture (50–150 °C), decomposition of hemicellulose and cellulose (200–350 °C), and lignin degradation (> 400 °C). SEM images showed rupture of the original surface and deposition of dispersed metallic particles. EDS analysis quantified a molybdenum oxide content of 16.31%, consistent with the precursor charge. Adsorption/desorption isotherms showed surface area, pore volume, and pore diameter of 118.7470 $m^2.g^{-1}$, 0.7366 $cm^3.g^{-1}$, and 11.2524 nm, respectively. Transesterification reactions were optimized using a factorial experimental design in a stainless steel reactor. The maximum yield of fatty acid methyl esters (99.5%) was obtained with a methanol/oil molar ratio of 45:1, 1.5% catalyst by mass, 190 °C and 1.5 h. Reuse tests showed good stability for up to five cycles and a yield of 78% after ten cycles. Thus, the catalyst achieved a 99.5% yield, with high stability over ten cycles, representing an efficient and low-cost route for biodiesel production.

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Performance of Cu–Co bimetallic Catalysts supported on Graphitic Carbon Nitride for Methanol Synthesis by CO_2 hydrogenation

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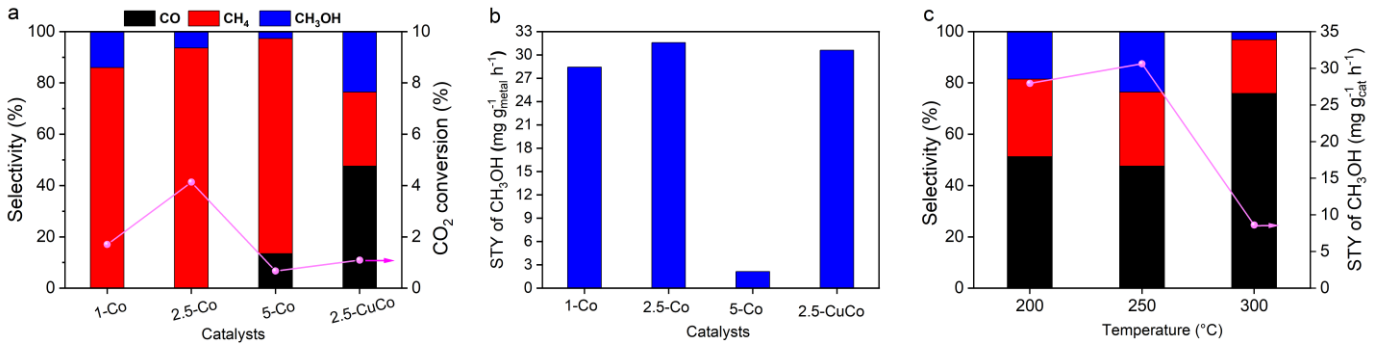
Palavras Chave:*CO2 Hydrogenation,Heterogenous Catalysis,Bimetallic Catalyst,Copper,Cobalt*

Highlights

Suppression of Methanation in CO_2 Hydrogenation over CuCo/g-C3N4 Intermetallic Catalysts Interfacial Engineering of Cu–Co Catalysts for Methanol Synthesis from CO_2

Resumo/Abstract

The continuous increase in carbon dioxide (CO_2) emissions and the adverse climatic impacts that arise from them urgently demand technological developments for the efficient catalytic conversion of CO_2 gas into value-added products. Among them, particular interest has been demonstrated for methanol (CH_3OH). Since Brazil completely depends on the importation of this strategic chemical, this project focuses on the development of an innovative heterogeneous catalyst based on bimetallic Cu-Co nanoparticles supported on graphitic carbon nitride (g-C_3N_4), aiming towards the selective hydrogenation of CO_2 to methanol while minimizing the formation of undesired byproducts, such as methane (CH_4). The synergistic effects of combining Cu and Co are being investigated, as well as the influence of the g-C_3N_4support on active site dispersion and catalytic performance. Our latest data suggest that the incorporation of both Cu and Co onto the g-C_3N_4 support enhances selectivity to CH_3OH (corresponding to 22% of products) while reducing methanation by 94%, simultaneously maintaining a satisfactory Space-Time Yield (STY) of 31 mgCH_3OH gc_{at}^{-1} h^{-1}. Thus, indicating that synergistic effects likely arise from the combination of the two metals. Temperature variation studies on the best performing catalyst (2,5-CuCo, where the numerical value represents the weight percentage of metal in relation to the support) revealed an optimal reaction temperature of 250 °C, as a higher temperature of 300 °C resulted in lower selectivity to CH_3OH and poor STY, and a lower temperature of 200 °C lead to a worse overall performance. Despite the general performance improvements provided by the bimetallic Cu-Co catalyst, conversion rates remained minimal, slightly lower than its monometallic Co counterpart. Future studies will be conducted towards further enhancements, namely, fine-tuning of the catalyst composition, addition of promoters such as Gallium, and comparative analysis of different supports.



a) Catalytic performance over catalysts b) Methanol Productivity of catalysts c) Temperature study

Agradecimentos/Acknowledgments

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Photocatalytic C–H Chlorination by Metal-Free Carbon Nitrides

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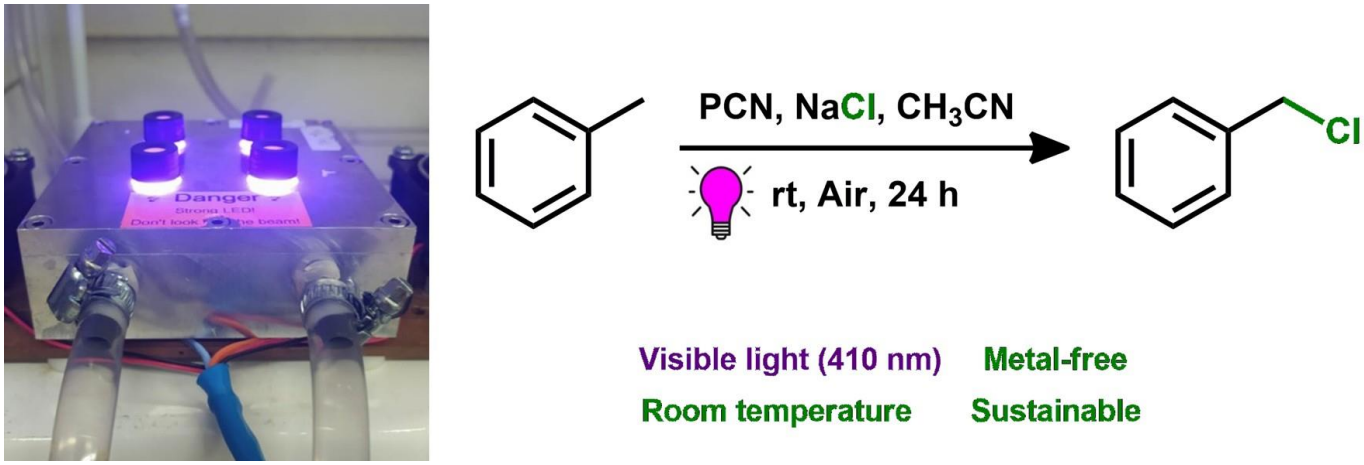
Palavras Chave:*Visible-light-driven C-H chlorination using NaCl and PCN; Sustainable, metal-free, and mild conditions; High selectivity (84.7%) and excellent conversion (97.8%) for chloroacetophenone.,Visible-light-driven C-H chlorination using NaCl and PCN; Sustainable, metal-free, and mild conditions; High selectivity (84.7%) and excellent conversion (97.8%) for chloroacetophenone.,Photocatalysis,C–H Chlorination,Metal-Free,Carbon Nitrides,Green Chemistry*

Highlights

Visible-light-driven C-H chlorination using NaCl and PCN; Sustainable, metal-free, and mild conditions; High selectivity (84.7%) and excellent conversion (97.8%) for chloroacetophenone.

Resumo/Abstract

Chlorinated compounds are essential to the chemical and pharmaceutical industries. However, traditional chlorination methods rely on chlorine gas (Cl_2), which is toxic, corrosive, and environmentally hazardous. Consequently, sustainable alternatives using NaCl as a low-cost chlorine source have gained attention. Since NaCl requires activation to overcome its low reactivity, photocatalysis emerges as a simple and effective strategy. In this work, polymeric carbon nitride (PCN) was employed as a sustainable and metal-free photocatalyst. Chlorination was achieved under mild conditions using visible light irradiation (410 nm), ambient air, and NaCl (36 mg) as the chlorine source in acidified acetonitrile (1 mL CH_3CN with 7 µL HCl). High selectivities of 84.7%, 74.1%, and 74.0% were obtained for 4-chlorobenzyl chloride, 4-nitrobenzyl chloride, and 1-phenylethyl chloride, respectively. Notably, benzyl chloride was obtained from toluene with 78.3% selectivity, and chloroacetophenone was synthesized from styrene with an excellent conversion of 97.8% and 74.0% selectivity.



Photocatalytic system for C-H chlorination using PCN and NaCl under visible light and ambient air.

Agradecimentos/Acknowledgments

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Photocatalytic CO2 reduction mediated by poly(heptazine imide)

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Palavras Chave:*Photocatalysis,Carbon Nitrides,CO2 Reduction,Heterogenous Catalysis,Poly(Heptazine Imide)*

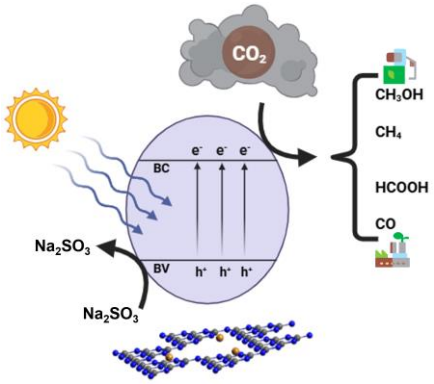
Highlights

Reduction of CO_2 into value added molecules under a photocatalytic system and mild conditions, utilizing a highly crystalline carbon nitride materials, poly(heptazine imide).

Resumo/Abstract

The CO_2 molecule is the most important greenhouse gas on Earth, responsible for aiding in regulating the global temperature. However, anthropogenic generated CO_2 from fossil fuels burning has progressively increased this molecule concentration in the atmosphere, leading to rampant global warming and the current climate change crisis. One of the proposed ways to deal with CO_2 emissions is carbon capture and utilization (CCU). This approach relies on sequestering CO_2 from high emission sources and chemically converting it into usable chemicals and fuels (e.g. CH_3OH, CH_4, CO_2H etc.), however, one main hinderance to CCU is the high thermodynamic stability of CO_2.

Therefore, in this work, we have applied highly crystalline carbon nitrides, Poly(Heptazine Imide) (PHI), as photocatalysts for the reducing CO_2 reduction reaction (CO_2RR) under mild conditions. The preparation of PHI involves the mechanical mixing of melamine and NaCl (1:10 wt/wt), followed by a thermal treatment under N_2 atmosphere, yielding Na-PHI. In the Na-PHI structure, Na^+ cations can be exchanged by being dispersed in a solution containing different metal ions yielding M-PHI (M = Fe, Ni, Co etc.), which can enhance the photocatalytic capabilities of the original material. In photocatalytic experiments we've applied both Na-PHI and different M-PHI for the CO_2RR. Results showed in pressurized vessel (~6 bar of CO_2) that Na-PHI can reduce CO_2 directly to CH_4 (0,030 $\mu mol.g^{-1}.h^{-1}$). When screening Ni-PHI materials with different loading we observed that Ni-PHI 0.5% had the highest reaction rate with main products being CO, CH_4 and H_2, followed by Ni-PHI 2% producing only CH_4. When applying Ni-PHI 2% at higher pressure, it was three times more efficient (0,85 $\mu mol.g^{-1}.h^{-1}$) than Na-PHI but generated H_2, which is a competitive side-product. These results, while modest, showcase the capabilities of PHI-based material being applied to CO_2RR in low pressure systems, and using only light as energy input.



Schematic representation of the photocatalytic reduction of CO2 by carbon nitrides

Agradecimentos/Acknowledgments

The authors would like to thanks the funding from CAPES, CNPq, FAPESP (process nº 2024/12042-4), and FINEP.

Photo-Enhanced Hydrogen Transfer Catalyzed by PN–Ruthenium Complexes

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Palavras Chave:*Transfer hydrogenation,photocatalysis,ketone reduction,ruthenium complexes*

Highlights

Ru complexes act as efficient photocatalysts for ketone reduction using isopropanol; Photo-enhanced transfer hydrogenation of ketones using PN–Ru complexes at mild conditions.

Resumo/Abstract

Transfer hydrogenation (TH) is a valuable strategy for the reduction of unsaturated organic substrates, relying on hydrogen donation from readily available sources such as isopropanol or formic acid, thus avoiding the use of molecular hydrogen. Although traditional TH processes often demand elevated temperatures and high energy consumption, photoinduced transfer hydrogenation has gained increasing attention as a more efficient and sustainable approach, offering new opportunities for the development of greener catalytic systems. Complexes 1–2 were synthesized through the reaction of $[Ru(\eta^2\text{-}OAc)_2(PPh_3)_2]$ with phosphine–pyridine (PN) ligands in methanol. These ruthenium complexes were evaluated as photocatalysts for transfer hydrogenation of ketones, using isopropanol as the hydrogen donor and NaOiPr as the base at 30 °C. Irradiation of the samples was carried out by using a 300 W Xenon Arc Lamp (LSB530 A, LOT-Oriel, Darmstadt, Germany), emitting in the range 200–2500 nm (solar simulator). We performed a screening using different ketone substrates to evaluate the complex. Complexes 1 and 2 exhibited comparable photoinduced behavior, showing low activity under dark conditions but significantly enhanced catalytic performance upon light irradiation. Notably, complex 1 was completely inactive in the absence of light, highlighting the essential role of photoactivation in its catalytic mechanism.

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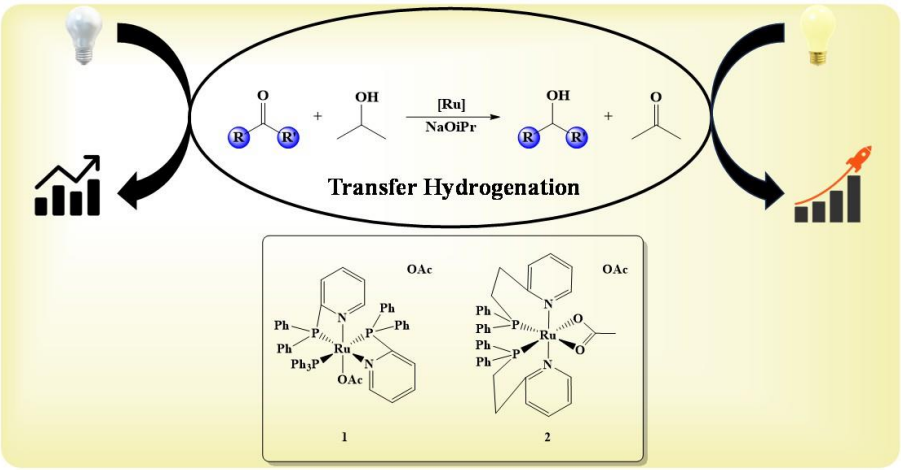


Photo-transfer hydrogenation catalyzed by 1 and 2.

Agradecimentos/Acknowledgments

Fundação de Amparo à Pesquisa do Estado de São Paulo - FAPESP (Proc. 2024/15926-0, 2022/12417-2, and 2021/13128-1);

Síntese, caracterização e potenciais aplicações catalíticas de hidroxinitrato de cobre(II)

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Palavras Chave:*Porphyrin,Layered hydroxide salts,Heterogeneous catalysis,oxidation reaction*

Highlights

Synthesis and characterization of layered solid copper(II)hydroxy nitrate salt (HNC) via controlled co-precipitation method and preliminary investigation as catalyst for oxidation of 1,5-DHN.

Resumo/Abstract

As porfirinas e metaloporfirinas (MP) são modelos biomiméticos versáteis com aplicações em catálise e fotocatálise. Devido à alta seletividade na oxidação de substratos orgânicos, o emprego de MP em sistemas heterogêneos é eficaz para aumentar a robustez e facilitar a recuperação do catalisador. Os Hidroxissais Lamelares (HSL) destacam-se como suportes promissores, constituídos por íons divalentes (M^{2+}) coordenados a hidroxilas, gerando lamelas que abrigam ânions hidratados na região interlamelar ou coordenados à lamela. Este trabalho descreve a síntese de um HSL de cobre(II) para imobilização de MP ou como catalisador. O sólido foi obtido por coprecipitação sob agitação, utilizando solução aquosa $Cu(NO_3)_2 \cdot 3H_2O$ (0,33 mol/L) com adição gota a gota de amônia aquosa (10 mol/L) sob controle de pH, chegando até pH 7,01 a 23 °C. A caracterização do hidroxinitrato de cobre(II) (HNC) azul foi realizada por FTIR, MEV, DRX e UV-VIS. O sólido foi investigado como catalisador na oxidação do 1,5-diidroxinaftaleno (DHN) para produção de Juglona em água, à temperatura ambiente e sob irradiação de luz branca (4 lâmpadas de 25 W), mantendo a proporção catalisador (Cu^{2+})/substrato (DHN) em 1:10. Resultados preliminares indicam que o borbulhamento de ar sintético é essencial: na presença do gás, houve acréscimo de cerca de 50% na formação do produto em relação à ausência de atmosfera de ar. Na sequência, o HNC será utilizado para imobilização de metaloporfirinas de diferentes íons metálicos, visando preparar sólidos eficientes para diversas reações catalíticas.

Agradecimentos/Acknowledgments

CAPES, CNPq, Fundação Araucária e Instituto Nacional de Ciência e Tecnologia em Ciências Moleculares (INCT-CiMol), Projeto CNPq 406804/2022-2.

Síntese Simplificada de Nanocubos Ocos de Pd–Cu2O para Evolução Eletrocatalítica de Hidrogênio em Meio Alcalino

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Palavras Chave:*HER,Nanobowls,Substituição galvânica,Eletrocatálise,Cu2O-Pd*

Highlights

Pd–Cu_2O hollow nanobowls obtained via galvanic replacement; Catalyst withenhanced HER activity with lower overpotentials and favorable kinetics; Performance similar or improved compared to Pt/C.

Resumo/Abstract

O trabalho apresenta a síntese de nanobowls ocos de Pd–Cu_2O por um método em duas etapas que combina o processo poliol e a reação de substituição galvânica, na qual esferas de Cu2O atuam como templates sacrificiais e agentes redutores para a deposição de Pd, resultando em arquiteturas bimetálicas porosas com alta área superficial e sítios catalíticos acessíveis. A**Figura 1**(microscopia) evidencia a transformação morfológica das esferas sólidas de Cu2O em estruturas ocas após a reação galvânica, confirmando a formação de nanobowls com organização porosa e domínios interconectados — características diretamente associadas ao aumento da área ativa e ao favorecimento do transporte de massa. As análises estruturais revelaram contração do parâmetro de rede e deformações interfaciais decorrentes da incorporação de Pd, indicando forte integração entre as fases e possíveis melhorias na transferência de carga e na adsorção de hidrogênio. Nos testes eletrocatalíticos para a reação de evolução de hidrogênio em meio alcalino, os nanobowls exibiram desempenho superior ao Cu2O puro, com menores sobrepotenciais, cinética mais favorável e elevada estabilidade, além de se aproximarem — e, em altas densidades de corrente, superarem — o desempenho do Pt/C comercial. Assim, os resultados demonstram que os nanobowls de Pd–Cu_2O apresentam um equilíbrio competitivo entre atividade, durabilidade e eficiência, configurando-se como uma alternativa promissora e potencialmente escalável aos catalisadores à base de platina para a produção sustentável de hidrogênio.

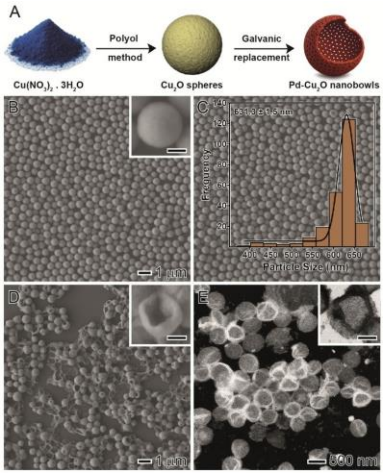


Figura 1: Esquema da substituição galvânica e MEV/MET evidenciando a formação dos nanobowls.

Agradecimentos/Acknowledgments

Agradecemos à FAPERJ, CNPq e CAPES pelo apoio financeiro.

Silica-Encapsulated Nickel Oxide Catalysts for Gas-Phase Hydrogenation of Furfural

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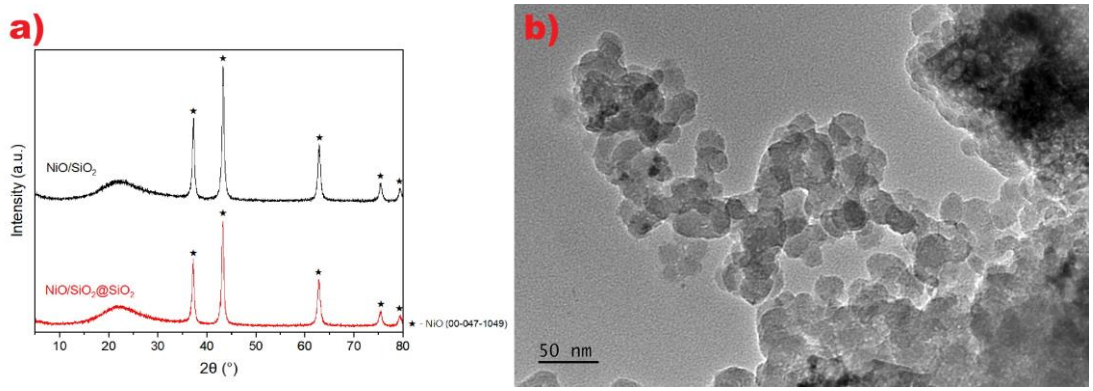
Palavras Chave:*nickel-based catalysts, heterogeneous catalysis, furfural hydrogenation, core@shell,core-shell,furfural hydrogenation,heterogeneous catalysis,,nickel-based catalysts*

Highlights

Development of innovative core@shell nickel-based catalysts; utilization of lignocellulosic biomass residues in biorefinery processes; promotion of low-cost and sustainable catalytic system.

Resumo/Abstract

The increasing demand for energy and the environmental impacts associated with fossil fuels intensified the search for renewable and sustainable alternatives for fuel and chemical production. In this context, this work addressed the development of nickel oxide–based catalysts supported on silica and encapsulated in silica core@shell structures for the gas-phase hydrogenation of furfural, aiming at the valorization of lignocellulosic biomass within a biorefinery framework. Nickel was employed as a low-cost and efficient active metal. The NiO/SiO_2 sample was synthesized by a solvent-free mechanochemical method for 1 h and subsequently calcined at 350 °C for 2 h. The $NiO/SiO_2@SiO_2$ sample was prepared using NiO/SiO_2, CTAB, and TEOS to form the silica shell, followed by calcination at 350 °C for 4 h. Fourier Transform Infrared Spectroscopy (FTIR) analysis identified characteristic bands associated with the angular deformation vibrations of Si–O–Si and Si–OH bonds at approximately 1080 cm^{-1} and 800 cm^{-1}, respectively, as well as a vibration attributed to Ni–OH species around 475 cm^{-1} [1]. X-ray diffraction (XRD) patterns (Figure a) revealed characteristic diffraction peaks of NiO at 2θ = 37.31°, 43.34°, and 62.98° [1], along with the broad amorphous halo typical of SiO_2, confirming the incorporation of nickel oxide into the silica matrix. Transmission Electron Microscopy (TEM) (Figure b)analyses showed a well-defined spherical morphology with an average particle diameter of approximately 50 nm. Energy-Dispersive X-ray Spectroscopy (EDS) confirmed the homogeneous distribution of nickel species and the successful formation of the core@shell architecture. Overall, the results demonstrated the potential of these materials for the upgrading of biomass-derived platform molecules.
[1] Sumithra, S. & N. Victor Jaya.*J. Supercond. Nov. Magn.*,**30**(2017) 1129–1136.



(a) XRD patterns of the NiO/SiO_2 and $NiO/SiO_2@SiO_2$ samples and (b) TEM images of the $NiO/SiO_2@SiO_2$.

Agradecimentos/Acknowledgments

We acknowledge the financial support from FAPESB and thank the partner laboratories (LAMUME, GCP, and CATAM) for technical support and infrastructure.

Sodium Alginate as Catalyst Support for CO2 Cycloaddition to Epoxides

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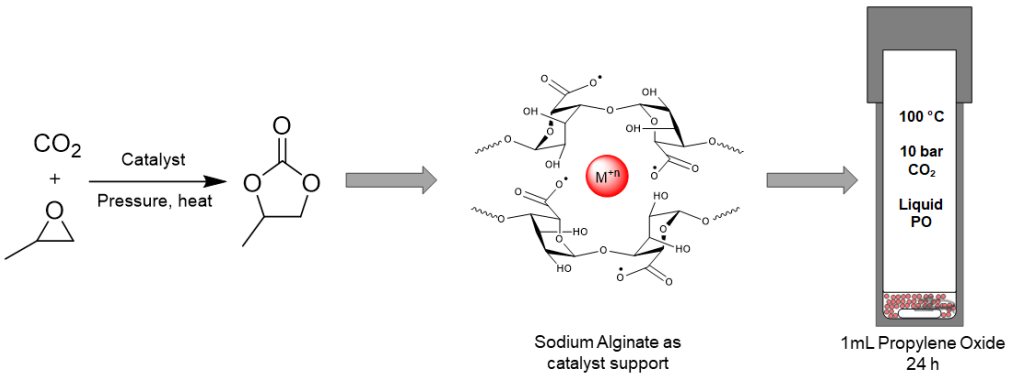
Palavras Chave:*Sodium Alginate,Heterogeneous Catalysys,Propylene Carbonate,CO2 Cycloaddition,Hydrogel*

Highlights

Heterogeneous catalysis of CO_2 cycloadditon to epoxides shows advantages for the industry. Sodium alginate is a known polimer for catalyst support, and shows potential of heterogenization of TBAB.

Resumo/Abstract

The cycloaddition of CO_2 to epoxides is a well-established route for the synthesis of cyclic carbonates, with GHG emissions mitigation potential. Sodium alginate has been widely explored in the literature as a versatile support for heterogeneous catalysts. To the best of our knowledge, its application as a support in CO2/epoxide cycloaddition systems has not been reported. This work therefore evaluates the performance of lyophilized sodium alginate hydrogel beads as catalyst supports for representative catalytic systems in this reaction. Efficient CO_2 cycloaddition typically requires the cooperative action of Lewis acidic and Lewis basic sites. Three supported systems were investigated: (i) Fe(III), (ii) Fe(III) combined with polyethylenimine (PEI), and (iii) a TBAB–Zn(II) system, all immobilized within the alginate bead matrix. While Fe(III) and PEI–Fe(III) showed limited yield and selectivity, both systems demonstrated promising mechanical characteristics for potential operation in packed-bed configurations. In contrast, the TBAB–Zn(II) system delivered satisfactory yield and selectivity, consistent with prior literature reports. Since TBAB is typically employed as a homogeneous catalyst, its immobilization on alginate offers an strategy to simplify phase separation and enable catalyst recovery, representing a relevant proof-of-concept for future developments. Material characterization indicated extensive crosslinking in the Fe(III) system and possible crosslinking disruption in PEI–Fe(III), with both materials exhibiting comparatively brittle behavior. By contrast, TBAB–Zn(II) alginate beads displayed high mechanical integrity, including strong tearing resistance despite significant deformability, and effective Zn retention after reaction. Future work will focus on improving catalytic performance, including evaluation of TBAB retention after reaction, optimization of phase homogenization to reduce mechanical stress, and systematic catalyst recycling studies.



Graphical Abstract - Simplified Representation of Reaction Conditions and Catalytic Support Employed

Agradecimentos/Acknowledgments

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Stability of Rh-Induced Subsurface Oxygen Vacancies on CeO_2(111): Structural and Energetic Implications

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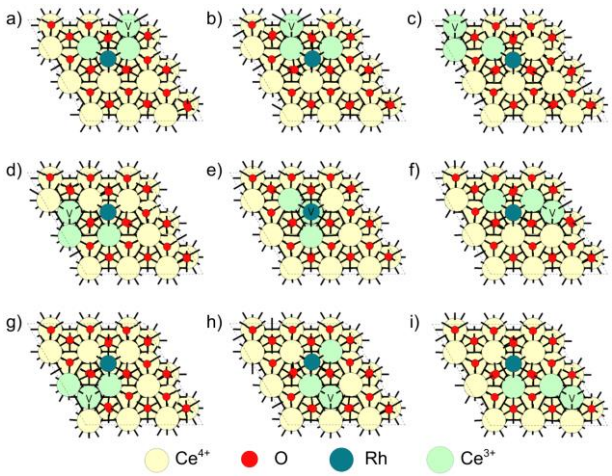
Palavras Chave:*Subsurface vacancy,CeO_2(111),DFT,Catalysis*

Highlights

Energy stability of subsurface oxygen vacancies was investigated for the Rh/CeO_2 system using DFT.

Resumo/Abstract

Cerium oxide (CeO_2) is widely studied as a catalytic support due to the presence of structural defects on its surface, particularly oxygen vacancies, which play a fundamental role in molecular activation [1]. The introduction of transition metals on the CeO_2(111) surface can further modify the stability of these vacancies as well as the electronic properties of the system [2]. In this work, nine distinct subsurface oxygen vacancy sites in the Rh/CeO_2(111) system were investigated through computational calculations based on Density Functional Theory (DFT), performed using the Quantum ESPRESSO package, as illustrated in Figure 1.
A CeO_2(111) (3×3) slab containing three O–Ce–O layers was constructed, with the bottom layer kept frozen during the geometry optimizations. Initially, the subsurface oxygen vacancy formation energy was calculated for the pristine CeO_2 slab, yielding a value of approximately 1.96 eV, in good agreement with literature data [3]. Subsequently, the nine subsurface vacancy configurations shown in Figure 1 were evaluated. It was observed that only configurations d, e, and g exhibited vacancy formation energies higher than that of the metal-free system, whereas configuration c led to the greatest stabilization of the vacancy, with a formation energy of 1.63 eV. Additionally, the adsorption energy of the Rh atom becomes more favorable in the presence of the vacancy, following the same trend observed for the vacancy formation energy. These results highlight the strong dependence of subsurface oxygen vacancy stability on its position relative to the metal, emphasizing the role of Rh in modulating the properties of the Rh/CeO_2 system.



CeO_2(111) slab containing a Rh atom and nine distinct subsurface oxygen vacancy configurations.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP (Grant No. 2021/00675-4), CNPq (Grant Nos. 301923/2025-6 and 132241/2025-0), and CAPES.

Statistical Optimization of Ni/CeO2 Catalysts for High CO2 Methanation Conversion

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Palavras Chave:*CO2 methanation,Ni/CeO2,Design of Experiments,Central Composite Design,Heterogeneous catalysis*

Highlights

CCD and RSM enable ration optimization of Ni/CeO_2 catalysts;
Ni loading and reaction temperature dominate catalytic performance;
Optimized catalyst achieves 92% CO_2 conversion and 100% CH_4 selectivity.

Resumo/Abstract

The catalytic conversion of CO_2 into methane via the Sabatier reaction is a promising route for carbon capture and utilization, particularly in Power-to-Gas systems. However, catalyst synthesis is still largely based on empirical trial-and-error approaches, where variables such as metal loading, calcination temperature, and reaction conditions are varied independently. This methodology neglects interaction effects, requires numerous experiments, and often leads to suboptimal and poorly reproducible catalysts. In this context, Design of Experiments (DoE) enables the identification of significant variables, evaluation of interactions, and simultaneous process optimization. Herein, a Central Composite Design (CCD) combined with Response Surface Methodology (RSM) was applied to optimize Ni/CeO_2 catalysts for CO_2 methanation. The effects of Ni loading, calcination temperature, and reaction temperature on CH_4 production rate and CO_2 consumption were systematically investigated. Catalysts were synthesized by coprecipitation and tested in a fixed-bed reactor under continuous flow. Experimental data were fitted to second-order polynomial models and evaluated by ANOVA. The models showed high statistical significance, coefficients of determination above 0.98, and no significant lack of fit. Ni loading and reaction temperature were the most influential factors, while calcination temperature had a secondary effect. Response surfaces revealed optimal regions governed by the balance between kinetic effects and thermodynamic limitations of the highly exothermic methanation reaction. An optimized catalyst containing 10 wt.% Ni and calcined at 500 ºC achieved 92% CO_2 conversion, 100% CH_4 selectivity, and an apparent activation energy of 73.67 kJ mol^{-1}, confirming the robustness of the statistical approach.

Agradecimentos/Acknowledgments

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Study of the stability and reactivity of PdnB clusters for the semi-hydrogenation of alkynes

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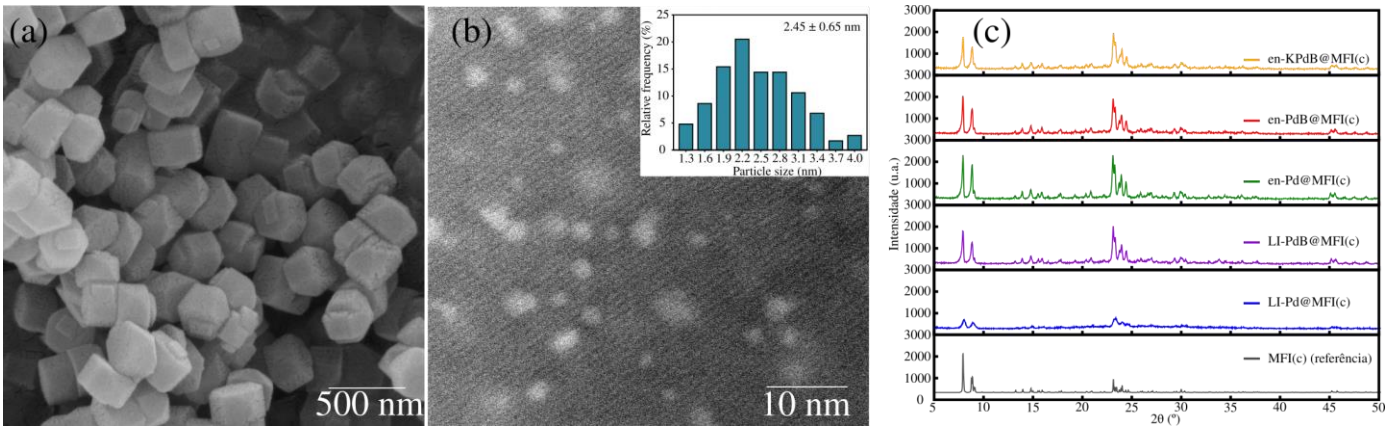
Palavras Chave:*semi-hydrogenation,MFI,catalysis,palladium-boron,clusters*

Highlights

One-pot synthesis of Pd_nB clusters for semi-hydrogenation.
B-doping as modulation against over-hydrogenation.
Subnanometric Pd_nB species in MFI topology with potential for selectivity.

Resumo/Abstract

Palladium nanoparticles and clusters play an essential role in heterogeneous catalysis, especially in selective semi-hydrogenation of alkynes. However, with the ease formation of beta-hydride (β-PdH_x) located in tetrahedral and octahedral sites of palladium clusters formation, these materials face a catalytic challenge in avoiding over-hydrogenation. This study explores the synthesis of palladium clusters encapsulated within MFI zeolite frameworks, aiming for structural and electronic modulation for catalytic alkyne hydrogenation. A one-pot synthetic strategy was employed, utilizing bis(ethylenediamine)palladium(II) ($Pd(en)_2Cl_2$ -noted as "en") and/or 1-butyl-3-methylimidazolium tetrachloropalladate (BIMPd - noted as "LI") with 1.0 % of silicon mass as precursors. The core approach involves incorporating boron into the zeolitic lattice to induce the migration of B atoms during calcination at 600 ºC, potentially forming interstitial Pd–B alloys. Characterization via X-ray diffraction (XRD), scanning electron microscopy (SEM) confirmed the maintenance of the MFI topology and transmission electron microscopy (TEM) to the size of bimetallic clusters. Preliminary results indicate that Pd is highly dispersed as subnanometric clusters or isolated atoms, with Pd_nO_m species forming upon calcination, as evidenced by the TEM images with average size of (2.45 ± 0.65) nm. These preliminary findings suggest that B-doping is a viable strategy for modulating Pd clusters, and ongoing catalytic tests aim to demonstrate the potential of these materials in suppressing over-hydrogenation pathways, thereby enhancing selectivity in alkyne transformations.



Results of en–PdB@MFI: (a) SEM; (b) TEM and histogram; and (c) XRD for the other species.

Agradecimentos/Acknowledgments

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Sugarcane Bagasse Lignin Hydrogenolysis: Competitive Ethanol Reforming over Cu-Doped Mixed Metal Oxides

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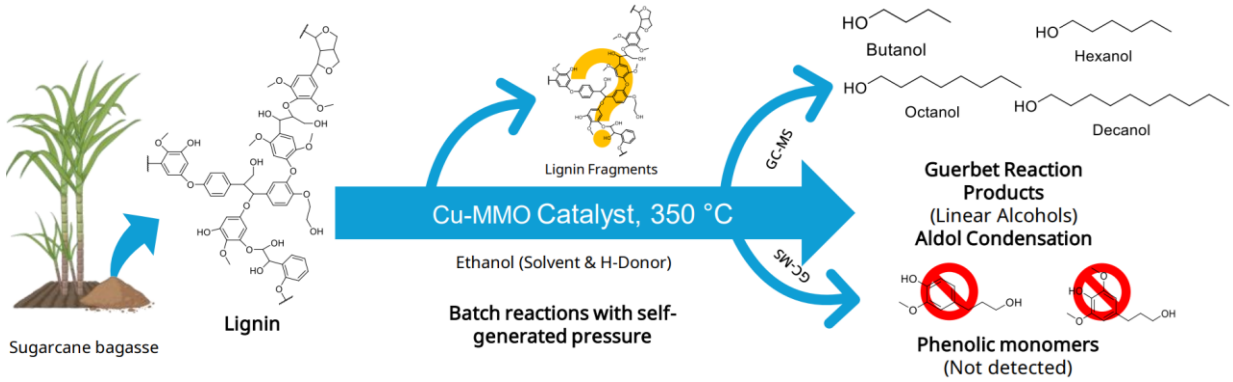
Palavras Chave:*Lignin,Sugarcane Bagasse,Mixed Metal Oxides,Guerbet Reaction,Hydrogenolysis*

Highlights

Cu-doped MMOs derived from hydrotalcites favored ethanol Guerbet reaction over sugarcane bagasse instead of lignin hydrogenolysis, yielding C4-C10alcohols.

Resumo/Abstract

Sugarcane bagasse is a major agro-industrial residue in Brazil and a strategic source of lignin to produce renewable aromatic chemicals. This work evaluated the catalytic depolymerization of sugarcane bagasse lignin via hydrogenolysis using Cu-doped Mixed Metal Oxides (MMO) derived of hydrotalcites (HTC). The lignin was isolated through alkaline extraction and characterized by Fourier-Transform Infrared Spectroscopy (FTIR) and X-ray Diffraction (XRD), confirming its amorphous nature and functional groups. The HTC, catalysts precursors, were synthesized by co-precipitation (Mg^{2+}/Al^{3+} molar ratio 3:1) doped with Cu (10 and 20 mol% substitution of Mg^{2+}) and MMO were obtained calcining HTC at 450 °C for 5h.
XRD analysis of MMO confirmed the successful formation of the periclase-like solid structure. Catalytic tests were realized in batch reactors at 350 °C using ethanol as solvent and hydrogen donor. Gas chromatography–mass spectrometry (GC-MS) analysis of the volatile fraction did not reveal phenolic monomers. Instead, a homologous series of linear alcohols (butanol, hexanol, octanol, decanol) were identified. These results indicate the dominance of the Guerbet reaction instead of hydrogenolysis, where Cu-based active sites promoted ethanol dehydrogenation followed by aldol condensation.
The absence of lignin monomers suggests strong kinetic competition where solvent reforming prevailed over lignin hydrogenolysis. In conclusion, while the synthesized Cu-MMOs demonstrated high catalytic activity for alcohol upgrading, the hydrogenolysis conditions require optimization. Also, liquid chromatography–mass spectrometry (LCMS) analysis will be further carried out to check if lignin oligomers were obtained during the catalytic reactions. Future studies will focus on evaluate lignin extracted through organosolv methods and employing alternative solvents, such as methanol, to mitigate competitive reactions and enhance depolymerization.



Formation of linear alcohols via Guerbet reaction over Cu-MMO.

Agradecimentos/Acknowledgments

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Surface Switch for Nickel Anchoring and Selectivity Control in Nitrobenzene Reduction

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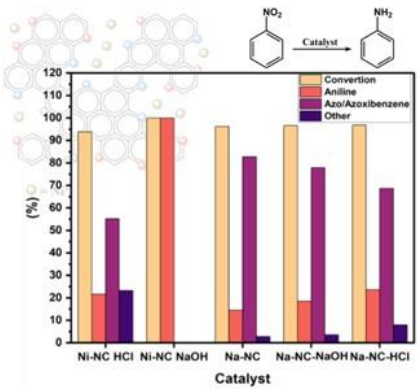
Palavras Chave:*Nitrogen-doped carbon, nickel, surface treatment, nitrobenzene reduction,Nitrogen-doped carbon,nickel,surface treatment,nitrobenzene reduction*

Highlights

Simple synthesis yields N-doped carbon with negatively charged surface sites
NaOH treatment enables controlled Ni incorporation by ion exchange
High conversion and selectivity in nitrobenzene reduction

Resumo/Abstract

A nitrogen-doped carbon (Na-NC) was synthesized by thermal treatment of cellulose as the carbon source, in the presence of NaCl and hydrolyzed collagen as the nitrogen source, aiming at the generation of negatively charged sites on the support. After purification, the material was subjected to post-synthetic treatments with 1 M HCl or NaOH solutions for 1h at room temperature to modulate the surficial groups, by protonation or deprotonation. Subsequently the samples were modified via an ion exchange with Ni^{2+} performed at room temperature. ICP-OES quantification evidenced a strong influence of the chemical treatment on metal incorporation: the untreated material incorporated 0.12 wt% of Ni, the NaOH-treated material exhibited a significantly higher Ni content (0.63 wt%), whereas the acid-treated sample showed Ni contents below the detection limit, indicating suppression of metal anchoring. These results indicate that the deprotonation of surface functional groups promoted by alkaline treatment is a key factor for the stabilization of Ni species on the N-doped carbon support.The catalytic activity was evaluated in the reduction of nitrobenzene using $NaBH_4$ as the reducing agent. All materials exhibited conversions above 90%; however, marked differences in product selectivity were observed. The Ni-NC NaOH catalyst showed high selectivity toward aniline, evidencing the role of incorporated Ni in promoting complete hydrogenation of the nitro group. In contrast, Ni-free materials favored partial reduction pathways, leading predominantly to coupling products such as azoxybenzene and azobenzene. These results demonstrate that controlled Ni incorporation not only enhances catalytic efficiency but also directs reaction selectivity. It can therefore be concluded that a N-doped carbon material can be synthesized through a simple and scalable route, in which mild surface treatments enable controlled of Ni, and consequently tuning the product selectivity to nitrobenzene reduction



Ni/N-doped carbon as an efficient catalyst for the conversion of nitrobenzene to aniline.

Agradecimentos/Acknowledgments

We acknowledge the financial support from FAPESP (Grant No. 2023/12949-7), Capes, CNPq, FINEP, and the LabIvo research group.

Surfactant-assisted crystallization: Increasing zeolite crystallinity with mechanochemical activation

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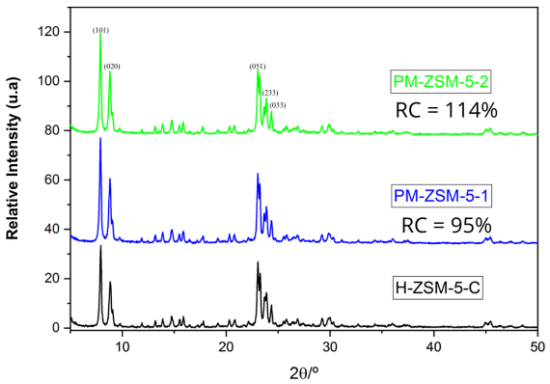
Palavras Chave:*Mechanochemistry,Crystallization,Zeolite,ZSM-5,Ball milling*

Highlights

High-energy ball milling promoted crystallite size growth instead of structural amorphization. XRD analysis confirmed enhanced long-range ordering and increased relative crystallinity.

Resumo/Abstract

Zeolites are microporous aluminosilicates widely used in adsorption and catalysis. Conventional high-energy ball milling (HEBM), commonly employed to reduce particle size, often causes crystallinity loss and structural collapse. In this study, the mechanochemical activation of a commercial ZSM-5 zeolite in the presence of structure-directing agents (SDAs), hexadecyltrimethylammonium bromide (CTAB) and tetrapropylammonium bromide (TPABr) was carried out using 1g of zeolite and 20 milling balls (6 mm diameter) for 20 min at a rotational speed of 500 rpm. The ZSM-5 precursor was subjected to HEBM using a Retsch PM-200 planetary ball mill. Structural properties were evaluated by X-ray diffraction (XRD), with crystallite size estimated using the Scherrer equation and relative crystallinity (RC) determined by peak integration. Fourier transform infrared (FTIR) spectroscopy was performed in the 4000–400 cm^{-1} range. XRD results revealed an unexpected increase in diffraction peak intensities after milling. Activation with CTAB resulted in a decrease in RC to 95%, whereas the combined use of CTAB and TPABr increased RC to 114%, indicating enhanced crystallinity relative to the original ZSM-5 sample. The Scherrer analysis showed peak narrowing at full width at half maximum (FWHM), corresponding to an increase in crystallite size from 40.8 nm to 46.3 and 46.9 nm. Contrary to the fragmentation typically associated with HEBM, these results indicate crystallite growth. This behavior is attributed to a mechanochemical-assisted recrystallization process, in which HEBM combined with interfacial stabilization provided by SDA, promotes the reorganization of superficial amorphous regions or oriented nanocrystalline domains into more ordered structures with reduced defect density and improved long-range alignment. FTIR confirmed framwork reinforcement via SDA and mechanochemical activation of the zeolite. Lastly mechanochemistry offer a promising strategy for crystallization of zeolites



X-ray diffraction patterns of mechanochemically activated ZSM-5 without and with SDA

Agradecimentos/Acknowledgments

The authors acknowledge financial support from the National Council for Scientific and Technological Development (CNPq, Brazil; Project No. 312461/2022-4) and the Coordination for the Improvement of Higher Education Personnel (CAPES, Brazil).

Synthesis and catalytic application of magnetic γ-Fe_2O_3/MEL zeolite composite for dephosphorylation

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Palavras Chave:*Zeolite,Catalysis,Dephosphorylation,Magnetic nanoparticles*

Highlights

Magnetic γ-Fe_2O_3/MEL composite for efficient dephosphorylation Achieved 10^4 catalytic acceleration towards organophosphate degradation Reusable catalyst for environmental organophosphorus degradation

Resumo/Abstract

A novel one-pot synthesis was developed to obtain a magnetic γ-Fe_2O_3/MEL zeolite composite, in which iron oxide nanoparticles are uniformly dispersed within a nanosized pure-silica MEL framework. Iron oxide-filled carbon nanotubes were employed as an efficient hard template, while TBAOH acted as a structure-directing agent, promoting the formation of the desired zeolitic architecture. The successful synthesis and structural integrity of both pristine MEL zeolite and the FeCNT@MEL composite were confirmed through comprehensive characterization using X-ray diffraction (XRD), X-ray Absorption Near Edge Structure (XANES), and micro-XRF mapping. XRD patterns revealed the presence of well-defined nanocrystalline zeolitic domains, indicating high structural order and phase purity. XANES analysis identified maghemite (γ-Fe_2O_3) as the predominant iron species after calcination, which is directly responsible for the composite's magnetic properties. This magnetic behavior enables rapid and efficient catalyst separation and recovery from reaction media using an external magnetic field, significantly improving operational efficiency and catalyst reusability. The composite exhibited remarkable catalytic performance in dephosphorylation reactions, a key process for the degradation of environmentally hazardous organophosphorus compounds, including pesticides and nerve agent simulants. At pH 8.5, the catalyst promoted an acceleration of approximately 10^4-fold in the degradation of 2,4-dinitrophenyl diethyl phosphate compared to spontaneous and conventional alkaline hydrolysis. Moreover, the material maintained high catalytic activity over multiple consecutive cycles, demonstrating excellent stability and robustness. These results highlight the strong potential of this magnetic zeolite composite as an efficient, reusable heterogeneous catalyst for environmental remediation and organophosphorus detoxification applications

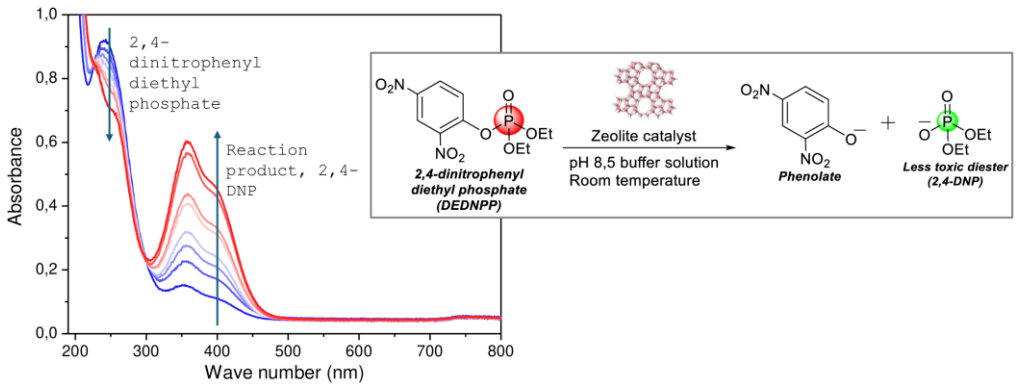


Figure 1. Schematic representation of the catalytic dephosphorylation reaction and kinetic plots mon

Agradecimentos/Acknowledgments

The authors thank UFPR, CAPES, CNPq, INCT Nanovida, and INCT Nanocarbono for their invaluable financial and institutional support, which was crucial for the development of this research.

Synthesis and characterization of ZIF-8 structures based on Zn2+ and Ni2+ and modified by amine ligand for CO2 reduction.

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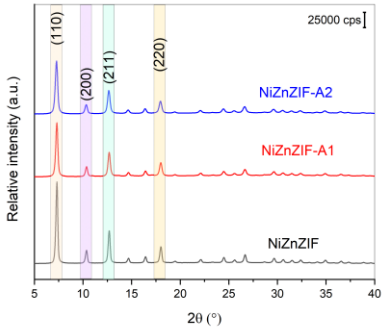
Palavras Chave:*ZIF-8,MOFs,greenhouse effect,morphology,crystal structure*

Highlights

Study of the morphology and structural properties of ZIF-8 for the reduction of atmospheric CO2, after modifications to its structure, through the use of Zn2+ and Ni2+ and hexadecylamine ligand.

Resumo/Abstract

Removing carbon dioxide, one of the main greenhouse gases in the atmosphere, has become one of the greatest environmental challenges facing humankind in the 21st century. Since the beginning of the industrial era in the 18th century, human activities have increased atmospheric CO2 by 50%. So Carbon capture and storage (CCS) technologies are considered essential as a short- to medium-term solution to minimize the impact of global warming until renewable technologies reach the necessary maturity. In recent years, zeolitic imidazolate frameworks (ZIFs) have developed rapidly. Their structures are generated according to tetrahedral units where each metal ion is linked to four organic imidazolate ligands. ZIFs are considered a subfamily of MOFs, and their topology has been similar to that of zeolites. Furthermore, ZIFs are considered attractive candidates for various applications, a benefit attributed to their excellent properties, including high surface areas, microporous structures, chemical and thermal stability, and synthesis controllability. ZIF-8 is composed of 2-methylimidazole ligands and a metal has been widely explored in diverse areas. ZIF-8 is also characterized by its ability to retain its crystallinity and porosity. Furthermore, the pore size and structure of ZIF-8 are easily adjustable, making it suitable for modification. Thus, in this work, ZIF-8 was modified using Ni2+ to increase the active sites of the structure, a fact that causes pore clogging. To overcome this factor, the hexadecylamine ligand (HDA) is used to increase its affinity for the CO2. Finally, this work aims to explain the synthesis and characterization of ZIF-8 structures to verify if it is possible to produce these structures by incorporating nickel and HDA into their composition, while still maintaining the structural characteristics that guarantee the efficiency of these structures, especially in reducing atmospheric CO2.



XRD of ZIF-8: NiZnZIF (Ni^{2+}), NiZnZIF-A1 (12.5% HDA) and NiZnZIF-A2 (25% HDA).

Agradecimentos/Acknowledgments

The authors thank FAPESP for funding the research and UNESP (Faculty of Sciences, Bauru campus) for the infrastructure provided.

Synthesis, Characterization, and Adsorptive Performance of Ni2+/Zn2+ Bimetallic ZIF-8 Functionalized with Hexadecylamine for CO2 Capture

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Palavras Chave:*ZIF-8,Nickel,Heterogeneous Catalysis,Hexadecylamine,CO2 Adsorption*

Highlights

The ZIF-8 containing Ni^{2+} was synthesized;The molar ratio of $Ni^{2+}/(Ni^{2+}/Zn^{2+})$ was 0.8;Ni-doped ZIF-8 exhibit higher CO_2 adsorption than pristine ZIF-8.

Resumo/Abstract

In recent decades, there has been growing concern about the excessive accumulation of carbon dioxide (CO_2) in the atmosphere and its profound impact on the global environment, as this gas is one of the contributors to global climate change. Zeolitic imidazolate frameworks (ZIFs) have been intensively investigated for their potential to capture CO_2. ZIFs are subclasses of structures that arise from MOFs, Metal-Organic Frameworks, and have attracted significant studies in catalysis, gas adsorption, gas separation, etc. Originally, ZIF-8 is a structure synthesized in the presence of Zn^{2+} as a cation. The partial replacement of Zn^{2+} by Ni^{2+} is an attempt to associate the adsorption capacity of CO_2 of the ZIF-8 structure with the catalytic potential of Ni^{2+}. However, this substitution may reduce the material porosity, since Ni^{2+} tends to form octahedral geometries, whereas Zn^{2+} adopts tetrahedral coordination. To compensate for this loss and enhance CO_2 adsorption, amines such as hexadecylamine (HDA) can be introduced, which chemically interact with CO_2through chemisorption. We synthesized the samples in molar proportion $Ni^{2+}/(Ni^{2+}/Zn^{2+})$ was 0.8, being a sample at room temperature in an autoclave for 24 hours. The samples containing HDA were designated with the letter 'A' (A1 = 0.0103 g of HDA and A2 = 0.0206 g of HDA). The methanol was the solvent, and the ligand was 2-methylimidazole. Figure 1 shows the result of CO_2 adsorption of samples. The NiZnZIF sample showed the highest CO_2 adsorption (0.040 g after 40 min), followed by the NiZnZIF-A1 sample (0.035 g after 40 min), both outperforming pristine ZIF-8, which exhibited a CO_2 uptake of 0.010 g after 40 min, whereas the NiZnZIF-A2 sample showed the lowest adsorption capacity (0.005 g after 40 min). These results demonstrate that Ni incorporation significantly enhances the CO_2 adsorption performance of ZIF-8, while excessive hexadecylamine loading negatively affects the adsorption capacity.

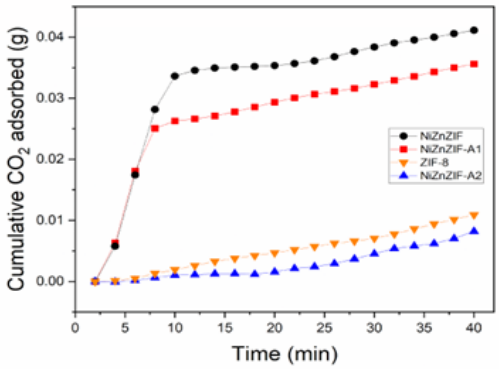


Figure 1. Cumulative CO2 adsorbed of samples ZIF-8, NiZnZIF, NiZnZIF-A1, and NiZnZIF-A2.

Agradecimentos/Acknowledgments

The authors thank the funding bodies FAPESP, CAPES CNPq, and the Brazilian Chemical Society.

Synthesis of CdS and $Zn_xCd_{1-x}S$ Photocatalysts Supported on Lucina pectinata Seashell Powder for Solar Hydrogen Generation

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Palavras Chave:*Heterogeneous photocatalysis, Solar hydrogen, CdS, $Zn_xCd_{1-x}S$, Waste valorization*

Highlights

Seashell waste was used as a support for sustainable photocatalytic semiconductors.

The support and Zn^{2+} promoted stability, efficiency, and sustainability in hydrogen production.

Resumo/Abstract

The search for clean and sustainable energy sources has driven the development of new technologies, particularly solar hydrogen production. A promising approach involves water splitting through photocatalytic processes using semiconductors. Among these materials, metal sulfides, especially cadmium sulfide (CdS), stand out due to their high visible-light absorption; however, their application is limited by photocorrosion and cadmium toxicity. In this context, this work proposes the deposition of CdS and $Zn_xCd_{1-x}S$ solid solutions onto seashell powder from the mollusk*Lucina pectinata*(“lambreta”), a marine solid waste mainly composed of $CaCO_3$ in the aragonite phase. In addition to mitigating improper disposal of coastal residues, the use of this support adds value to an abundant material in coastal communities and enhances the scalability of the photocatalytic process. Results obtained by XRD, Raman spectroscopy, and EDS confirmed the formation of the expected phases, good dispersion of the semiconductors on the support, and structural changes consistent with $Zn_xCd_{1-x}S$ alloy formation. SEM analyses revealed homogeneous morphologies, while Raman spectra indicated interactions between CdS and the carbonaceous matrix, associated with enhanced structural stability. Among the evaluated samples, the semiconductor-to-support ratio of 1:5 (ZnCdSL15) exhibited the best performance, achieving a hydrogen production rate of 3973.3 μmol g^{-1} h^{-1}, comparable to or higher than values reported in the literature. The incorporation of Zn^{2+} and chemical anchoring to the $CaCO_3$ support significantly increased semiconductor stability, mitigating photocorrosion under prolonged irradiation. Recycling tests confirmed the durability and reproducibility of the material, highlighting its potential for sustainable H_2 generation and for the energy transition with reduced local environmental impacts.

Agradecimentos/Acknowledgments

The authors acknowledge CNPq and FAPESB for financial support, SEC-BA for granting the license, and IQ-UFBA for institutional support.

Synthesis of copper(II) cyclodextrin complex and its catalytic application towards the synthesis of diarylamines via Chan-Lam reaction.

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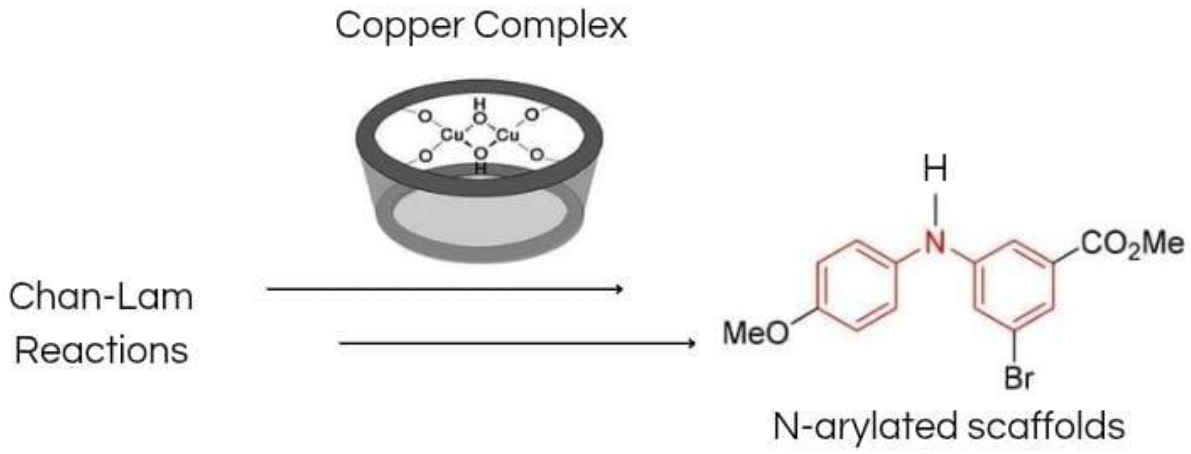
Palavras Chave:*Chan-Lam reaction, β-cyclodextrin, copper, mechanosynthesis,Chan-Lam reaction, β-cyclodextrin, copper, mechanosynthesis*

Highlights

Copper(II) β-cyclodextrin complex was synthesized in solution and in solid state; Its catalytic activity was evaluated in the preparation of a model diarylamine via Chan-Lam reaction in water.

Resumo/Abstract

About 90% of all electric energy generated in Brazil comes from hydro and thermoelectric plants. Due to the climate emergency, national energy sovereignty requires mastery of solar thermal energy technologies. Carbazole derivatives are interesting alternatives for the 3rd generation dye-sensitized solar cells due to low precursor cost, good charge transport capacity and ease of functionalization. Within this context, this work investigates the C-N cross-couplings - key to obtaining a number of DSSC scaffolds - in the copper catalyzed Chan-Lam reaction in water. In this case, the catalytic activity of a copper(II) β-cyclodextrin complex was investigated in the reaction between phenylboronic acid and p-anisidine, as a model. The complex was obtained from 2 synthetic routes - in solid and aqueous phase. Mechanochemical synthesis attempts occurred using precursors $CuSO_4$, β-CD and KOH performed in a Retsch ball mill apparatus, operating at 20 Hz for 1 or 2h. Moreover, the stoichiometry was evaluated in ratios of 2:1:3 or 2:1:6 (metal:CD:base). In addition, ultrasound-activated catalytic tests were used at 45ºC for 6h. The wet route reaction occurred according to the Kaboudin procedure [2]. The navy blue solid obtained was characterized by DRS, FTIR and TGA. DRS analyses of the wet route showed the expected d-d transitions band at 676 nm. However, this band was not so clearly observed in the solid state. XRD results showed a low degree of crystallinity followed by slight intensity changes and peak shifts. Additional characterization is underway in order to investigate the complex formation in solid state. The catalytic reactions with p-anisidine showed moderate to good yields towards the product N-phenyl-p-anisidine under ultrasound (60-70%), especially with time increasing. By contrast, control tests with reaction precursors did not show conversion. The scope of the reaction along with the ultrasound effect are ongoing.



Synthesis of diarylamines catalyzed by Cu and β-CD complex via Chan–Lam Reaction

Agradecimentos/Acknowledgments

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Synthesis of novel ionic organocompounds and their application in solvent-free CO2 cycloaddition to propylene oxide

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Palavras Chave:*CO2 conversion,, cyclic carbonates,cyclic carbonates,green chemistry*

Highlights

The conversion of CO_2 into value-added products is a key challenge. In this study, two novel catalysts synthesized via a simple route are proposed.

Resumo/Abstract

The increase in atmospheric CO_2 levels is a major concern due to its contribution to the greenhouse effect. In this context, the cycloaddition of CO_2 to epoxides to form cyclic carbonates is particularly relevant, as it converts a potential pollutant into high value-added products[1]. These cyclic carbonates are polar aprotic solvents with important applications in the pharmaceutical and agrochemical industries. This study investigates novel ionic organocompound catalysts (OC1 and OC2, Figure 1) as potential systems for this reaction. Their halide counteranions can promote epoxide ring opening via nucleophilic attack, while organic functionalities such as imidazole rings and amine groups may facilitate CO_2 activation through Lewis basic interactions and stabilization of reaction intermediates. Both compounds were synthesized through a simple procedure by stirring the reactants in isopropanol overnight. OC1 was prepared at room temperature, whereas OC2 required heating to 80 ºC. After solvent removal and drying under reduced pressure, OC1 was obtained using a 2.2:1 molar ratio of 1,2-dimethylimidazolium to 1,2-bis(bromomethyl)benzene, affording an 82.8% yield. OC2 was synthesized using a 3:1 molar ratio of triethylamine to 1,2-bis(bromomethyl)benzene and further purified in acetonitrile, yielding 54.8%. Both organocompounds were characterized by ^1H and ^{13}C NMR spectroscopy, confirming their purity. CO_2 cycloaddition reactions were carried out at 150 °C for 24 h under 15 bar in a batch reactor. Gas chromatography analysis showed that OC1 achieved a 74.7% yield and 96.3% selectivity toward propylene carbonate, while OC2 reached an 80.2% yield and 97.5% selectivity (Table 1). These results highlight the potential of ionic liquid-like organocatalysts as efficient and tunable systems for CO_2 cycloaddition to epoxides.

[1] WEN, T.T. et al. ACS Applied Materials & Interfaces, v. 17, n. 28, p. 40574–40582, 1 jul. 2025.

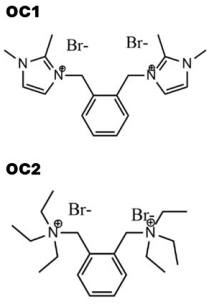
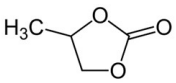


Figure 1: Organocompound Catalysts 1 (above) and 2 (below).

Desired product: 

Catalyst	Yield to PC (%)	Selectivity to PC (%)
OC1	74,7	96,3
OC2	80,2	97,5

Table 1: Catalytic results for the CO_2 cycloaddition into epoxides reaction, carried at 150 °C for 24 h under a pressure of 15 bar, using a batch reactor.

Structure of studied catalysts and catalytic results table.

Agradecimentos/Acknowledgments

The authors thank CNPq, Universidade Federal do Paraná, Fundação Araucária and SETI for the scholarship, infrastructure and the support through the Productivity Fellowship in Research and/or Technological Development.

Theoretical insights into the mechanism of the synthesis of coumarins using aminated cellulose-based catalysts

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Palavras Chave:*biomass,density functional theory,solvent-free,heterogeneous catalysis,organocatalysis.*

Highlights

Coumarins were produced in free-solvent conditions.

Conversion rates of 12.5-100% were achieved.

Two different reaction mechanisms were assessed from a molecular modelling perspective.

Resumo/Abstract

Coumarins can be synthed via the Knoevenagel condensation between ethyl acetoacetate (EAA) and hydroxybenzaldehydes. Here, three different aminated cellulose-based materials were investigated as sustainable heterogeneous catalysts for coumarin synthesis, combining experimental studies with density functional theory (DFT) calculations (Geerlings et al., 2003) to elucidate their catalytic behavior and reaction mechanisms. The catalysts were prepared by functionalizing microcrystalline cellulose with ethylenediamine, diethylenetriamine or N,N'-bis(2-aminoethyl)-1,3-propanediamine, enabling evaluation of how amine structure influences catalytic efficiency. Experimental results demonstrated that all materials catalyze the Knoevenagel reaction under solvent-free conditions. Computational modeling at the DFT level was employed to investigate two competing catalytic pathways: (i) an acid–base mechanism involving proton abstraction from EAA, and (ii) a pathway involving nucleophilic attack on the aldehyde and formation of iminium intermediates. Our calculations revealed that direct carbanion formation via simple acid–base reaction is energetically unfavorable. Frontier molecular orbital (FMO) analysis and reaction energy calculations indicated that secondary amines are the most active catalytic sites and that iminium formation can be thermodynamically viable. Simulated IR spectra supported experimental FTIR data, providing evidence for iminium intermediates during catalysis. Substituent effects on benzaldehydes were rationalized through molecular electrostatic potential and FMO analyses. Overall, the combined experimental and DFT results demonstrate that aminated cellulose-based materials are effective and sustainable catalysts for coumarin synthesis, and that computational chemistry can provide molecular-level insight into their reactivity, selectivity and catalytic mechanisms.
Geerlings, P. et al. (2003). Chemical Reviews, 103(5), 1793–1874. https://doi.org/10.1021/cr99002

Agradecimentos/Acknowledgments

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Thermally driven single-atom incorporation into the ceria lattice unlocks highly CO-selective CO2 hydrogenation

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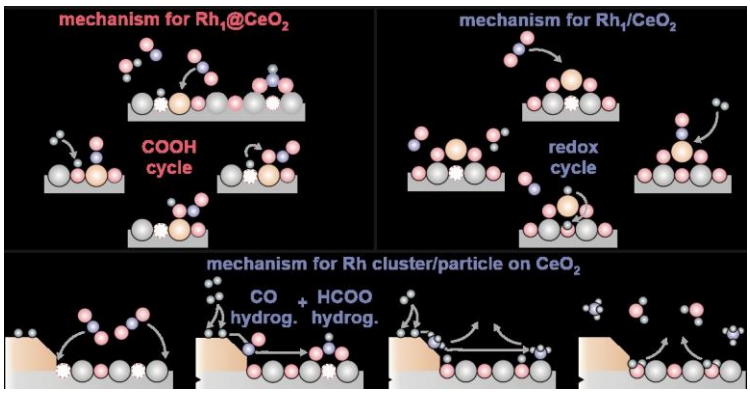
Palavras Chave:*single-atom,reverse water-gas shift,atom-trapping,catalyst design*

Highlights

High-temperature calcination stabilizes lattice Rh single atoms on CeO_2, suppressing aggregation and methanation, and enabling near-unity CO selectivity in CO_2 hydrogenation.

Resumo/Abstract

The selective hydrogenation of CO_2 to CO via the reverse water–gas shift (rWGS) reaction is a key challenge due to competition with methanation under thermodynamically favorable conditions. This study shows that thermal treatment critically influences Rh speciation on CeO_2, thereby affecting reaction selectivity. Catalysts with Rh loadings from 0.1 to 1.0 wt.% were prepared through strong electrostatic adsorption and then calcined at either a mild temperature (400 °C) or a high temperature (800 °C). Structural and spectroscopic analyses indicated that mild calcination mainly produced surface-supported Rh single atoms, which can partially cluster into metallic groups under reducing environments. In contrast, high-temperature calcination facilitated the integration of Rh into the CeO_2 lattice, resulting in highly stable, lattice-substituted Rh single atoms that remained isolated even in H_2-rich environments. Catalytic tests revealed that the lattice Rh sites achieved nearly 100% selectivity for CO across a broad temperature range. Meanwhile, catalysts with Rh aggregates tend to produce CH_4 as a result of improved H_2 dissociation and spillover. Kinetic analysis and site-specific turnover frequencies show that rWGS activity is directly related to the surface density of isolated Rh sites, and the product selectivity depends on site evolution, not on inherent reaction energetics. Mechanistic insights revealed that lattice-substituted Rh single atoms promote CO formation through a carboxylate pathway, while surface-supported Rh sites produce it via a redox mechanism. In contrast, Rh clusters and nanoparticles enable deep hydrogenation of strongly adsorbed formate and CO intermediates, ultimately producing CH_4. These findings demonstrate that thermal treatment is a versatile and effective approach for modifying metal-support interactions, stabilizing atomically dispersed active sites, and intentionally guiding selectivity in CO_2 hydrogenation on reducible oxide supports.



Proposed reaction pathways for CO2 hydrogenation on Rh-CeO2 catalysts as a function of Rh speciation

Agradecimentos/Acknowledgments

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Transformando o Coque em Aliado: Controle de Espécies Aromáticas Ativas em SSZ-13 para Melhoria da MTO

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Palavras Chave:*MTO,coque,zeólita*

Highlights

Controlled coking improves SSZ-13 MTO performance.

Coke favors active PAH formation.

Pre-coked catalyst deactivates more slowly.

Oxygenates modulate acidity at early stages.

CO_2 raises olefin selectivity.

Resumo/Abstract

A formação de coque em zeólitas é tradicionalmente associada à desativação catalítica. Neste estudo, essa visão é revisitada por meio da indução controlada de coque em catalisadores SSZ-13, visando melhorar o desempenho na reação de conversão de metanol em olefinas (MTO). A introdução de uma pequena quantidade de coque selecionado (1,6 % em massa), previamente identificada como ativa na MTO, foi utilizada para modular o ambiente catalítico. Durante a reação, hidrocarbonetos poliaromáticos (PAH) se formam no interior dos poros da zeólita e desempenham papel central no mecanismo da MTO. Enquanto espécies mais condensadas promovem desativação, PAH de menor tamanho favorecem a produção de olefinas. A formação de coque foi induzida com tolueno para controlar a geração dessas espécies. O catalisador pré-coqueado apresentou maior atividade inicial e uma taxa mais lenta de acúmulo inicial de PAH em comparação ao catalisador não modificado, resultando em menor desativação ao longo do tempo. A presença de pequenas quantidades de espécies oxigenadas nas etapas iniciais indica interações com os sítios ácidos da zeólita, capazes de modular a acidez e alterar a dinâmica da MTO. A adição de CO_2 como agente oxidante suave favoreceu a formação dessas espécies e promoveu um aumento de 10 % na seletividade a olefinas. Resultados de UV–Vis operando e análises por cromatografia acoplada à espectrometria de massas confirmaram a evolução controlada das espécies de PAH e do coque ao longo da reação.

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EDU - Ensino de Química

3D printed low-cost instruments developed for the popularization of chemistry teaching focused on Brazilian technological sovereignty.

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Palavras Chave:*STEAM,Democratization,Instrumentation,Technological sovereignty,3D Printing*

Highlights

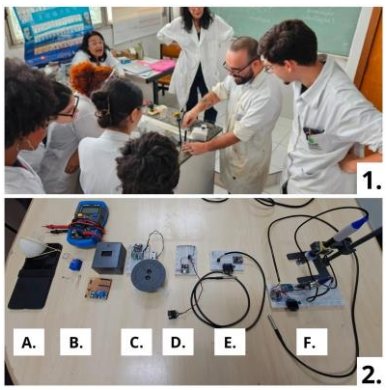
Development of basic analytical devices with an approximate cost of BRL 5.00 per student. Prototypes validated with precision equivalent to commercial equipment at 20–30% of market value.

Resumo/Abstract

The scarcity of financial resources and the high cost of precision equipment represent significant barriers to the consolidation of teaching and research laboratories. Given this scenario, this project aimed to develop low-cost and open-source analytical instruments — including pH meters, conductivity meters, turbidimeters, photocolorimeters, scales, and thermometers — integrating them into pedagogical practices of chemical analysis and environmental monitoring.

The selection of equipment was based on a previous survey of demands among teachers from IFRJ and UFRJ, spanning from elementary to higher education. The construction methodology involved prototypes with different levels of technological complexity, ranging from 3D-printed attachments for smartphones to perform turbidimetric and colorimetric measurements, to simple electronic components such as multimeters, LEDs, batteries, and photoresistors for conductivity, turbidimetric, and photocolorimetric measurements, as well as microcontrollers with specific sensors and display screens enclosed in 3D-printed parts for more precise physicochemical analyses equivalent to commercial products.

The practical application occurred through workshops and experimental classes at IFRJ (Nilópolis and Maracanã campuses), Naves do Conhecimento, and UFRJ, involving students from elementary to undergraduate and graduate programs in Science Teaching. In addition to technical validation, the project did a workshop at the Rio de Janeiro Science and Technology Festival, where five kits containing instruments without microcontrollers were donated to public school teachers. The results demonstrate that the construction of one's own devices, in addition to addressing infrastructure gaps, acts as a potent didactic strategy for the interdisciplinary teaching of electronics, analytical chemistry, and technological awareness concepts, while also stimulating student autonomy in building their own instruments to overcome everyday obstacles.



1: Workshop at UFRJ. 2: Prototypes (A-B: w/o microcontrollers; C-F: w/ microcontrollers).

Agradecimentos/Acknowledgments

I would like to thank IFRJ (CDUC, Nilópolis, and Maracanã campuses), Instituto Reditus, FAPERJ, CIEDS, and the Rio de Janeiro Municipal Secretariat of Science and Technology, which were fundamental for the funding, and application of this work.

A Área de Ensino de Química no Centro-Oeste Brasileiro (2005-2025): Um Supercrescimento Transformador

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Palavras Chave:*Área de Ensino de Química,Formação de Formadores,Região Centro-Oeste*

Highlights

The Chemistry Teaching Area in Central-Western Brazil grew by more than 1000% in terms of the number of active PhDs between 2005 and 2025, mainly due to local research groups.

Resumo/Abstract

O Ensino de química é uma área de pesquisa que investiga o aprendizado, produz conhecimento sobre formação docente e contribui para uma educação científica mais crítica, inclusiva e significativa. É uma área do conhecimento com crescimento vertiginoso, tanto no que se refere a artigos científicos, como a formação de mestres e doutores, principalmente nos últimos 20 anos.

Este trabalho apresenta como foi esse crescimento na Região Centro-Oeste do Brasil, em números de doutores com efetivo exercício nas instituições públicas e particulares no período 2005-2025. Como método, realizou-se uma pesquisa em sites de cada uma das instituições públicas ou privadas dos 4 estados da região Centro-Oeste (DF, GO, MS e MT), aliada à pedidos oficiais a todas as instituições, com efetiva resposta, por meio da ouvidoria federal, Fala.br, e cruzamento via plataforma Lattes, entre os meses de setembro a dezembro de 2025.

Os resultados mostram que houve o que denominamos de supercrescimento (mais que exponencial) de doutores no Centro-Oeste. O crescimento médio foi de 1150%. Em números absolutos, o Distrito Federal contava com 5 doutores/as em 2005. Em 2025, são 20 doutores/as (aumento de 300%). O Mato Grosso do Sul contava com 2 doutores em 2005. Em 2025, são 15 doutores/as (aumento de 650%). Em seguida, o Mato Grosso, que contava com 1 doutora. Em 2025, são 16 doutores/as (aumento de 1500%). Finalmente, o estado de Goiás, que contava com 2 doutores/as em 2005. Em 2025, são 45 doutores/as (crescimento de 2150%)

Este supercrescimento está relacionado, em sua maior parte, ao aumento e interiorização de programas de pós-graduação nas regiões Norte e Centro-Oeste, o que proporcionou que grupos de pesquisa da região fossem fortalecidos e formassem mais recursos humanos, e em menor escala a processos migratórios. Tal crescimento impactou no aumento expressivo de número de cursos de licenciatura em Química, formação de professores e melhoria do ensino de química em nível básico de ensino.

Agradecimentos/Acknowledgments

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A bioquímica por trás dos alimentos: inclusão a partir da aprendizagem por projetos

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Palavras Chave:*Educação inclusiva,Biomoléculas,funções orgânicas,alimentação e interdisciplinaridade,Educação Inclusiva*

Highlights

A inclusão é um pilar da educação.
Estudantes com deficiência permitem espaços de aprendizagem dinâmicos.
A Química e o cotidiano dos alunos no processo de ensino e aprendizagem.

Resumo/Abstract

A linguagem científica versus a linguagem cotidiana é um aspecto importante no ensino de Química na educação básica. A complexidade dos conceitos e a relação entre os níveis macroscópico, microscópico e simbólico representam grandes desafios no processo de Ensino de Química. A barreira entre estudantes e o conteúdo de química é ainda mais expressiva para estudantes com deficiências. Assim, o objetivo deste trabalho foi a realização do projeto “A Bioquímica por trás dos alimentos”, no qual os estudantes do ensino médio da escola SESI Blumenau, em equipes integrando estudantes com deficiência, apresentaram e produziram uma receita, relacionando o conteúdo de biomoléculas à culinária.

O trabalho foi desenvolvido nas disciplinas de Biologia e Química, em parceria com as professoras especialistas em atendimento aos alunos com deficiência de uma turma de primeiro ano. O projeto foi desenvolvido em 3 etapas: 1 - elucidação dos conceitos e divisão dos grupos; 2 - trabalho escrito e produção da apresentação; e 3 - produção da receita e apresentação oral. Os estudantes foram avaliados conforme os critérios: Observação Científica, Apresentação e Coesão e Qualidade do Prato. O trabalho escrito foi avaliado quanto à descrição de aspectos biológicos e químicos, ou seja, à identificação das biomoléculas, às suas ligações químicas e às suas funções orgânicas. Também foi avaliado o aspecto socioemocional, com foco no protagonismo e na colaboração dos estudantes. Por fim, foram avaliadas a entrega do prato e a degustação. Foi notável o envolvimento dos estudantes no projeto e a apropriação dos conceitos abordados. Além de realizar a atividade em grupos heterogêneos, houve envolvimento positivo com as famílias e os responsáveis.

O processo de ensino e aprendizagem, quando os estudantes colocam a “mão na massa” para construírem seu conhecimento com autonomia, incluindo seus pares e familiares nas atividades, é de grande impacto no processo educativo.



Apresentação final do projeto de biomoléculas do grupo que trabalhou fermentação biológica em pães.

Agradecimentos/Acknowledgments

Agradecimentos à FIESC e à escola SESI pela oportunidade de desenvolver o projeto e à FAPESC e à CAPES pela bolsa de mestrado.

Abordagem CTS a partir do Cultivo do Melão Gaúcho: o ensino de Química com foco na Realidade Local

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Palavras Chave:*CTS, Cultivo do melão Gaúcho.,Contextualização,CTS,Cultivo do melão Gaúcho*

Highlights

A miniconferência abordará a contextualização CTS no ensino de Química a partir de uma problemática envolvendo o cultivo do melão do gaúcho.

Resumo/Abstract

miniconferência iniciará com a apresentação dos pressupostos teóricos da abordagem Ciência, Tecnologia e Sociedade (CTS) no ensino de Química. A nossa compreensão converge com a de autores da área, os quais, em síntese, destacam que o objetivo do ensino é desenvolver atitudes e valores cidadãos nos estudantes por meio de articulações entre os conhecimentos da Ciência e da tecnologia e o contexto social. Na sequência, será apresentada a Unidade Temática (UT) desenvolvida em uma escola pública do município de Nova Santa Rita/RS, o qual é conhecido como um dos principais produtores de melão do estado. A construção do material didático partiu da realidade dos estudantes e da comunidade escolar, constituída por pequenos agricultores e trabalhadores do campo, os quais trouxeram a problemática do preço das folhas de jornais que, tradicionalmente, vêm sendo utilizadas em uma das etapas do cultivo do melão Gaúcho. A UT contemplou alguns conceitos de Química, por exemplo, elementos químicos, tabela periódica, íons, acidez e pH, relacionados a conhecimentos práticos de um produtor rural, parceiro da pesquisa, os quais proporcionaram a compreensão das etapas do cultivo do melão. Ademais, serão relatadas as atividades práticas desenvolvidas durante a aplicação da UT, tais como construção e manutenção de uma lavoura experimental na escola para o cultivo do melão Gaúcho, experimentos de análise de solo e desenvolvimento de materiais com potencial para substituir o uso das folhas de jornais na proteção dos frutos do melão. Os resultados obtidos indicam avanços na compreensão dos conceitos químicos relacionados ao cuidado do solo e cultivo do melão. Entre os materiais testados experimentalmente, destacou-se um produto obtido a partir de resíduos orgânicos, especialmente cascas de ovos, que se mostrou uma alternativa viável às folhas de jornal. Por fim, serão feitas considerações a respeito da importância da contextualização por meio da abordagem CTS.

Agradecimentos/Acknowledgments

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Acidificação dos oceanos no ensino de Química: uma proposta de experimentação fundamentada na Química Verde e na abordagem STEAM

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Palavras Chave:*Acidificação dos oceanos, Química Verde, Ensino de Química, Abordagem STEAM, Experimentação*

Highlights

Green Chemistry applied to science education.

STEAM education.

Real-time CO2 monitoring via Arduino.

Integrating STEAM and Green Chemistry.

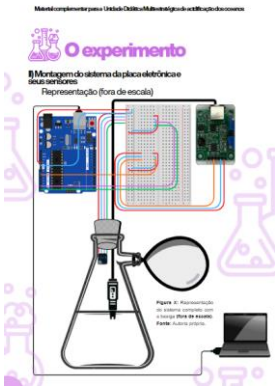
Green Chemistry for high schools.

Resumo/Abstract

A influência das emissões de CO2 na acidificação dos oceanos é reconhecida pela Organização das Nações Unidas (ONU) em seu 14º Objetivo de Desenvolvimento Sustentável (ODS 14). Segundo a ONU, os oceanos absorvem aproximadamente 23% das emissões globais de carbono. A Agenda 2030 define metas para mitigar esse fenômeno, destacando a importância do avanço científico como ferramenta para a conquista desses objetivos. Além disso, o estudo da acidificação dos oceanos também se relaciona aos 12 princípios da Química Verde, estabelecidos por Anastas e Warner (1998). Dentre os princípios, destaca-se o 11°: análise em tempo real para a prevenção da poluição, que fundamenta a proposta deste trabalho.

O objetivo deste trabalho foi a elaboração e avaliação de uma atividade experimental para o monitoramento de um processo de acidificação em ambiente laboratorial controlado, integrando conceitos curriculares do Ensino Médio brasileiro. A atividade fundamenta-se na abordagem STEAM (sigla em inglês para Ciência, Tecnologia, Engenharia, Artes e Matemática) e no Ensino de Ciências por Investigação. A proposta consiste na injeção de CO2 em um ambiente fechado no qual estão inseridos um conjunto de sensores de pressão, temperatura e pH conectados a uma a um computador e controlados via prototipagem com Arduino. Esse conjunto experimental permite o monitoramento em tempo real das variáveis e o estudo da influência do CO2 na acidificação da água.

Os dados dos testes experimentais mostram a possibilidade do estudo de conceitos de equilíbrio químico em nível básico e superior. A implementação da atividade com futuros professores resultou em engajamento e no desenvolvimento de conhecimentos associados à química e às disciplinas STEAM. Dessa forma, o projeto busca contribuir para além da inserção de temas contemporâneos e socialmente relevantes, uma vez que o experimento formulado permite a articulação de conhecimentos de diversas áreas, incluindo programação e tecnologia aplicada ao ensino.



Esquematização do experimento proposto.

Agradecimentos/Acknowledgments

À FAPESP, UNICAMP, Instituto de Química da UNICAMP, co.educa, Canal Futura — Fundação Roberto Marinho, CNPq, CAPES e ao programa Praticar Ciência.

A Divulgação Científica como Objeto de Mediação Pedagógica: Reflexões para o Ensino de Química sob a Ótica da Pedagogia Histórico-Crítica

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Palavras Chave:*saber sistematizado,prática social,popularização da ciência*

Highlights

O trabalho analisa a Divulgação Científica como mediação no Ensino de Química, utilizando a Pedagogia Histórico-Crítica para superar a consciência ingênua e acessar o saber científico sistematizado.

Resumo/Abstract

O presente trabalho propõe uma reflexão teórica sobre o papel da Divulgação Científica (DC) no Ensino de Química, distanciando-se de perspectivas que a reduzem a um mero recurso acessório, lúdico ou motivacional. O objetivo é discutir como a DC, ao ser tratada como um objeto de mediação pedagógica, pode atuar de forma estratégica para viabilizar o acesso dos estudantes ao saber científico sistematizado. A fundamentação teórica ancora-se nos pressupostos da Pedagogia Histórico-Crítica (PHC), que defende o ensino dos conhecimentos clássicos como ferramenta indispensável para a emancipação social, em diálogo com as teorias de comunicação de Wilson da Costa Bueno, que define a DC como um processo de recodificação de informações científicas para públicos não especializados. Metodologicamente, a pesquisa é de natureza qualitativa, do tipo bibliográfica e analítico-descritiva, centrada na análise de obras de referência que discutem a função social da escola e a comunicação da ciência. A análise foca, especificamente, na potencialidade da DC para as etapas de Prática Social Inicial e Problematização dos momentos pedagógicos de Saviani. Argumenta-se que, por possuir uma linguagem que transita entre o saber sistematizado e a prática social, a DC pode explicitar a visão sincrética dos alunos sobre os fenômenos químicos presentes na sociedade. No momento da Problematização, o material de DC pode atuar como um disparador de contradições, revelando que o conhecimento do senso comum é insuficiente para a compreensão total da realidade. Assim, a DC não é utilizada para tensionar a necessidade de apropriação do saber sistematizado, que será desenvolvido na etapa subsequente de Instrumentalização. Conclui-se que a integração da DC ao Ensino de Química, sob a ótica da PHC, fortalece a formação crítica ao transformar o fenômeno divulgado em objeto de estudo, promovendo a superação da consciência ingênua, essencial para a transformação da prática social do sujeito.

A importância da SNCT na formação de alunas do 9° ano do ensino fundamental como popularizadoras das ciências

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Palavras Chave:*Popularização da Ciência,Semana Nacional de Ciência e Tecnologia - SNCT,Mediação Científica,Empoderamento feminino,Biomas Brasileiros*

Highlights

Students from three state schools in Itápolis-SP, were challenged to create and present an exhibition about Brazilian biomes at the Municipal Museum at 21st National Science and Technology Week

Resumo/Abstract

A popularização da ciência pode ser entendida como o ato de divulgar, difundir a ciência para toda a comunidade, com o intuito, dentre outros, de combater a desinformação e tornar as informações complexas em acessíveis. Com o tema central biomas brasileiros, alunas de três escolas estaduais da cidade de Itápolis, SP, foram desafiadas a elaborarem e apresentarem uma exposição no Museu Municipal durante a 21° SNCT. Por seis meses, grupos de estudantes foram orientados por três professoras a pesquisarem e criarem objetos expositivos e, aos poucos, as alunas dos 9° anos do Ensino Fundamental foram entendendo a importância dos biomas, de uma forma interdisciplinar, aprendendo aspectos biológicos, geográficos e químicos de cada uma das regiões e, principalmente, as consequências das ações humanas. O objetivo do trabalho foi investigar a importância da SNCT como ferramenta motivacional na formação de popularizadores científicos. Durante a 21° SNCT, alunas voluntariaram-se para mediarem as visitas escolares. Os visitantes puderam ver maquetes, montar um quebra-cabeças formado por cubos e ler infográficos. Em três dias de atividades, a exposição recebeu 540 estudantes e após análise dos relatos das mediadoras, pode-se afirmar que elas aproveitaram a atividade e ficaram felizes em participar, como destacado na frase de uma das alunas, “a gente pode aprender mais sobre os biomas e repassar esse conhecimento para outras pessoas”, ou ainda “foi uma parte essencial na minha trajetória, pois eu realmente vi que eu tenho potencial para conseguir falar diante das pessoas, eu tinha muita dificuldade e lá, na frente de todo mundo, eu realmente consegui desenvolver, consegui apresentar o projeto.” Conclui-se que a execução do projeto e a SNCT foram de suma importância para que as alunas se tornassem protagonistas no processo de ensino-aprendizagem, desenvolvendo suas habilidades de pesquisa científica e transformando-as nas atrizes principais da popularização científica.



Alunos montando uma das faces do quebra-cabeças Biomas Brasileiros.

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A integração de posts do Instagram em um Estudo de Caso para identificar e desconstruir Desinformações sobre Plásticos Biodegradáveis

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Palavras Chave:*Estudo de Caso; Greenwashing; Redes Sociais; Educação Ambiental; Ensino de Química*

Highlights

Debunking greenwashing through investigative analysis of case study integrated to social media content. Development of argumentation and autonomy in Chemistry teacher education.

Resumo/Abstract

O cenário de pós-verdade e a disseminação da desinformação, potencializados no ambiente digital, demonstram a necessidade de que os futuros professores desenvolvam novas habilidades de análise crítica das informações. Neste contexto, o presente trabalho aborda uma intervenção pedagógica baseada na metodologia ativa de Estudo de Caso, realizada com licenciandos em Química da UFMS por meio do caso "O Lago da Dor". A pesquisa ocorreu em dois momentos. Primeiro, o pesquisador elaborou o caso seguindo os critérios de Sá e Queiroz (2010) e integrou à narrativa um perfil fictício no Instagram (@ecoplast_bio), que continha postagens com características de greenwashing e desinformação sobre polímeros. No segundo momento, os licenciandos de uma disciplina do curso investigaram a narrativa a fim de solucionar a problemática presente: a poluição do lago e a morte de animais no campus. Na sequência, os estudantes apresentaram, por meio da argumentação, a elucidação do caso e as soluções propostas. A análise qualitativa dos dados coletados evidenciou o trabalho colaborativo e a articulação da Química e Biologia com problemas locais e do cotidiano, além de os participantes relatarem autonomia na criação de hipóteses e no desenvolvimento de suas pesquisas. Entretanto, a intervenção expôs lacunas, como dificuldades na interpretação das informações e no acesso a fontes de materiais confiáveis na internet. Observou-se também que a identificação de algumas características de desinformação relacionadas aos polímeros e bioplásticos foi promovida somente após a discussão realizada, reforçando a importância do diálogo e a necessidade do letramento científico e midiático. Por fim, a articulação entre estudo de caso e rede social constitui uma abordagem alternativa para o ensino, podendo estimular habilidades para analisar e avaliar criticamente informações veiculadas por diversos meios, sejam eles físicos ou digitais, e integrar o combate à desinformação em práticas pedagógicas.

Agradecimentos/Acknowledgments

CAPES

Análise das estratégias argumentativas mobilizadas por especialistas em vídeos do YouTube de Divulgação Científica sobre Mudanças Climáticas

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Palavras Chave:*Mídias digitais, Argumentação, Educação em Química, Divulgação Científica, Análise Textual Discursiva,Mídias digitais,Argumentação,Educação em Química,Divulgação Científica,Análise Textual Discursiva*

Highlights

nArticulation between argumentation, digital media, and scientific literacy

Argumentative strategy analysis in videos about Climate Change

Misinformation challenges in digital science communication

Resumo/Abstract

As recentes transformações na esfera midiática digital têm reconfigurado modos de circulação e apropriação do conhecimento científico. Plataformas como o YouTube consolidaram-se como espaços de Divulgação Científica e de formação de opinião que, por vezes, podem ser usados por professores como recursos didáticos. Nelas, diferentes divulgadores científicos (DV) discutem temas de interesse público relacionados à ciência, o que pode influenciar a compreensão conceitual ou favorecer a desinformação.

Assim, o objetivo deste trabalho é compreender quais e como argumentos são mobilizados por DV em debates sobre Mudanças Climáticas em vídeos do YouTube. Para isso, os vídeos foram selecionados com base em critérios pré-estabelecidos, transcritos e, em seguida, analisados à luz da Análise Textual Discursiva. Por meio da categorização, identificamos e caracterizamos estratégias argumentativas empregadas pelos divulgadores.

Os resultados indicam que tais estratégias divergem conforme o posicionamento dos DV frente ao tema. Mesmo ao mobilizarem uma mesma categoria, como “Historicidade”, o discurso varia, produzindo efeitos persuasivos distintos, como a busca de apoio do público em vez de promover a compreensão conceitual. Observou-se também que aqueles que rejeitam ou relativizam as mudanças climáticas tendem a recorrer a argumentos voltados à deslegitimação de quem se pauta pelo consenso científico, deslocando o debate para disputas de credibilidade.

Consideramos, portanto, que a discussão sistemática de aspectos do discurso argumentativo deve integrar o currículo de Química e não se restringir a ações pontuais. Defendemos, assim, a instrumentalização dos alunos com ferramentas conceituais e argumentativas que lhes permitam não apenas compreender conhecimentos científicos, mas também posicionar-se de modo crítico e autônomo diante de informações duvidosas, fortalecendo sua alfabetização científica.

Agradecimentos/Acknowledgments

Agradece-se à Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) pelo apoio ao desenvolvimento desta pesquisa.

Análise das exposições e atividades educativas de Química do Centro de Ciências de Araraquara

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Palavras Chave:*Museus de Ciência,Divulgação científica,Exposições de Química,Interdisciplinaridade,Popularização da Química*

Highlights

New perspectives on the dissemination of Chemistry in science museums, integrating experimentation and educational games through exhibitions and educational activities that engage with other areas.

Resumo/Abstract

Museus e centros de ciências são espaços de educação não formal e divulgação científica, nos quais predominam exposições relacionadas às Ciência da Natureza. No Brasil, apenas 38% dos museus de ciência possuem exposições de Química, geralmente associadas ao “Show da Química” ou à exposição de objetos[1]. Palmieri e Silveira propõem três categorias para a divulgação da química em museus de Ciência: experimentação, por meio do cotidiano e interdisciplinar[2]. O Guia de Museus de Ciência e Tecnologia – SP (2024) lista 52 instituições, das quais apenas três relatam ter exposições de Química, destacando-se o Centro de Ciências de Araraquara (CCA) pela diversidade de abordagens apresentadas. Este trabalho caracteriza-se como uma pesquisa qualitativa, de caráter descritivo, que analisa as exposições e atividades educativas de Química desenvolvidas pelo CCA. O CCA conta com um laboratório de Química, onde são realizados experimentos do “Show da Química” durante visitas mediadas, além do Museu Histórico de Química, que abriga equipamentos históricos do Instituto de Química. A exposição “Primo Levi: um quimiscritor no museu” articula a química, literatura e história, enquanto a recente exposição “Química Verde: repensando a vida de forma sustentável” propõe uma abordagem inovadora, integrando painéis informativos, jogos interativos e experimentos. As oficinas formativas interdisciplinares voltadas ao público infantojuvenil promovem a interação com o laboratório e o acervo. A Figura 1 apresenta as exposições do CCA e suas categorias de divulgação química. A análise dos registros de visitação indica um aumento para 4.511 visitantes em 2025, evidenciando o potencial dessas ações na divulgação da Química em museus. Assim, o CCA se consolida como referência ao inovar nas estratégias de divulgação da Química em museus de ciências.
[1]Steola, A.C.S.; Kasseboehmer Química Nova, v.41, n.9, p.1072-1082, 2018.
[2]Palmieri, L.J.; Silveira, C. Revista Humanidades e Inovação, v.7, n.7, 2020.



Figura 1: Exposições de Química do CCA e suas categorias para a divulgação da Química.

Agradecimentos/Acknowledgments

Agradeço ao Centro de Ciências de Araraquara, ao Instituto de Química - UNESP e a PROEC - UNESP.

Análise do material de apoio do componente curricular de Química Aplicada fornecido pela SEDUC-SP

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Palavras Chave:*recursos didáticos,itinerários formativos,ensino de química,novo ensino médio*

Highlights

Os materiais de Química Aplicada da SEDUC-SP são organizados como trilhas de aprendizagem fortemente roteirizadas. Há baixa presença de referências científicas nos recursos didáticos disponibilizados.

Resumo/Abstract

A reorganização do Ensino Médio brasileiro, estabelecida pela Lei nº 13.415/2017 e pela BNCC, redefiniu a distribuição da Química no currículo ao dividi-lo em Formação Geral Básica e Itinerários Formativos[1] . No estado de São Paulo, a partir de 2024, a disciplina passou a integrar o itinerário de Ciências da Natureza no terceiro ano sob a denominação Química Aplicada, conforme a matriz curricular da SEDUC-SP [2]. Nesse contexto, este trabalho analisou os materiais de apoio docente fornecidos para esse componente, por meio de uma pesquisa qualitativa e documental. O material é estruturado em trilhas de aprendizagem organizadas em sequências que apresentam o tema, desenvolvem os conceitos e propõem atividades, funcionando como um roteiro previamente definido. Essa formatação reduz a margem de decisão do professor, ao estabelecer objetivos, conteúdos e recursos de modo padronizado, o que tende a limitar a autonomia pedagógica. Observou-se ainda que os conceitos químicos são abordados de forma pouco aprofundada, o que pode comprometer a consolidação dos conhecimentos necessários tanto para a continuidade dos estudos quanto para a inserção no mundo do trabalho. Além disso, a análise revelou a presença restrita de referências científicas, sendo frequente a indicação de vídeos da plataforma “YouTube” como principal fonte de complementação, o que fragiliza o rigor acadêmico do material. Esses resultados indicam que, embora os slides facilitem o planejamento, sua estrutura e base teórica apresentam limites que podem afetar a qualidade da formação científica dos estudantes.

Referências

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Análise dos experimentos propostos nos livros didáticos de química aprovados no PNLD 2026

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Palavras Chave:*Ensino de Química,Experimentação,Atividades Experimentais,Materiais Didáticos,Investigação científica*

Highlights

Avaliação das atividades experimentais em livros didáticos de Química do PNLD 2026, com foco nas abordagens metodológicas e em seu potencial para promover a investigação científica.

Resumo/Abstract

A experimentação exerce papel fundamental no ensino de Química ao articular teoria e prática, favorecer a compreensão dos fenômenos químicos e contribuir para o desenvolvimento de habilidades relacionadas à investigação científica escolar. Este estudo analisou as atividades experimentais presentes em livros didáticos de Química aprovados pelo PNLD 2026, totalizando 96 atividades experimentais distribuídas em 9 coleções.

As atividades experimentais foram classificadas em 6 categorias de acordo com a abordagem metodológica [1]: empírico-indutivistas, demonstrativas, ilustrativas, investigativas, conceituais e técnicas. A análise indicou a ausência de atividades empírico-indutivistas e pouca ocorrência de propostas demonstrativas e técnicas. Predominaram atividades ilustrativas, voltadas à exemplificação de conceitos, seguidas de atividades investigativas, que envolvem problematização, levantamento de hipóteses e análise de resultados. Os experimentos mais recorrentes abordam práticas de fácil execução, como a reação entre vinagre e bicarbonato de sódio, o uso de indicadores ácido-base, a medição de corrente elétrica e o estudo de fatores que influenciam a velocidade das reações químicas. As coleções “Moderna Plus”, “Identidade” e “Química por toda parte” apresentaram maior proporção de atividades investigativas, enquanto a coleção “Ciência Viva" concentrou o maior número de experimentos. O livro “Química 360º" apresentou apenas atividades ilustrativas e conceituais, e a coleção “InterAção" não apresentou experimentos, apenas uma sessão dedicada a projetos interdisciplinares.

Assim, os resultados indicam que a experimentação nos livros analisados concentra-se majoritariamente em atividades ilustrativas, enquanto as propostas investigativas aparecem de forma limitada e desigual entre as coleções, restringindo o envolvimento dos estudantes em processos de problematização.

1 Leite, B.S. Educación Química, v.29, n. 3, p.61-78, 2018.

Agradecimentos/Acknowledgments

Agradeço a Douglas Ricardo de Assis pela orientação e contribuições ao desenvolvimento deste trabalho, bem como ao Instituto de Química da UNESP de Araraquara pelo apoio institucional.

Analytical Limitations of Colorimetric Presumptive Tests in Forensic Drug Analysis: a purpose for forensic science communication.

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Palavras Chave:*Colorimetric assays,presumptive drug tests,forensic analytical chemistry,cross-reactivity,science communication*

Highlights

The goal was to critically assess the performance of traditional colorimetric tests for drugs of abuse while translating these insights into accessible educational content for society

Resumo/Abstract

Presumptive tests are commonly used in forensic drug analysis, especially in drug seizures. Among these methods, colorimetric assays remain prevalent due to their low cost and high sensitivity. However, from an analytical chemistry standpoint, their limited selectivity and high susceptibility to matrix effects create uncertainties. This work aimed to integrate reaction chemistry, interference phenomena, and the complexity of real samples to critically assess the analytical limitations of traditional colorimetric tests for drugs of abuse while exploring their potential as educational tools for teaching analytical chemistry concepts and promoting science communication. The study investigated the chemical mechanisms behind classical assays, including acid-catalyzed chromophore formation in the Duquenois–Levine test for THC detection and coordination complex formation in the Scott test for cocaine identification. Cross-reactivity with pharmaceuticals, plant-derived compounds, and structurally similar substances was demonstrated through controlled assays, highlighting false-positive results. The effects of common adulterants and diluents - including anesthetics, stimulants, sugars, and pharmaceutical excipients -were also examined to illustrate matrix effects and analytical interference. The experimental protocol was adapted into interactive demonstrations with high school students during outreach activities. Discussions on analytical reliability and forensic interpretation followed guided observation of the reactions. Learning outcomes were evaluated through brief questionnaires, indicating improved understanding of sensitivity, selectivity, specificity, and the limitations of presumptive tests. The findings reinforce the necessity of confirmatory methods for reliable drug identification and show that forensic analytical case studies can support teaching about chemical reactivity, analytical uncertainty, and critical interpretation of scientific evidence.

Agradecimentos/Acknowledgments

1. Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq INCT-SP: 406958/2022-0. 2. Programa Institucional de Bolsas (PUB), FFCLRP-USP. 3. Coordenação para o Aperfeiçoamento de Pessoal de Nível Superior: (CAPES, Financial Code 001).

An Analysis of Science-Related Denialist Discourses on TikTok: Perspectives for Science Education

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Palavras Chave:*Denialism,Fake News,TikTok*

Highlights

This work analyzes denialist discourses on TikTok about microwaves, using theories of denialism, hyperparticularization, and e-phemerality to explain their success and to propose counter-strategies.

Resumo/Abstract

This study proposes to analyze the content of the information tennagers are exposed to on this social network. The work began with data collection, searching for videos online on random days to obtain a representative sample. The initial focus was on videos regarding the effects of microwave ovens on food and health.

The second stage consisted of content analysis. A final corpus of 51 videos was selected and transcribed. This material was categorized into four groups based on predominant narratives: correct concept, loose concept, incorrect concept, and problematic explanations, with 21, 10, 7, and 10 videos, respectively. A fifth category (others) was created for videos that did not fit the primary groups (3). We observed that the "correct concept" category contains the highest number of videos (21). However, an analysis of the discourses reveals the presence of hyper-particularized concepts. Thus, even a technically correct concept, if isolated from its context, can lead to the spread of misinformation.

Tennagers face difficulties in fact-checking and, due to specific biases, end up finding information that, while correct, is decontextualized. This contributes to the creation of virtual bubbles with this type of content. Such exposure can transform them into spreaders of misinformation, both online and offline. To combat this phenomenon, the solution must go beyond simple fact-checking, which is limited to the accuracy of the content. It is fundamental that strategies evolve to focus not only on what is said, but above all, on the context in which the information is conveyed. This empowers the public to recognize and resist disinformation, even when it appears disguised as a correct concept.

Representative excerpts	
Category	**Excerpt**
Incorrect Concept (IC) (7)	"Por que o microondas é ruim? Por causa da energia eletromagnética. Ele **muda a composição do alimento, ele mata as propriedades nutricionais, ele acaba com as propriedades nutricionais**." (IC4)
Loose Concept (LC) (10)	"Mas o que serve micro-ondas, então? Para jogar fora. Comida morta, adulterada, totalmente sem vida. Esquentar um pedaço de carne no micro-ondas não é o mesmo produto que entrou. O que vai sair é diferente do que entrou. É o eletrodoméstico mais cancerígeno do planeta. Aposente o seu micro-ondas quanto antes. Se você quiser ter saúde." (LC5) "Os médicos não querem que você descubra essa verdade. Para cada problema no seu corpo, existe uma frequência que pode te curar. O próprio Nikola Tesla disse, se você quer encontrar os segredos do universo, pense em termos de frequência." (LC6)
Correct Concept (CC) (21)	"O micro-ondas é a energia elétrica transformada em energia eletromagnética." (CC2) "Por que o micro-ondas você não consegue abrir a porta enquanto ele está ligado? É para não escapar os raios." (CC2) "Você não pode esquentar nenhuma fórmula infantil em mamadeira de plástico no microondas. Isso é veneno. Isso é crime. Você está dando uma mamadeira de veneno para uma criança, depois não entende porque a criança está cheia de problemas, então isso tem que ser abolido, nada de plástico no microondas." (CC14)
Problematic Explanations (PE) (10)	"Há várias formas de carregar o corpo, como aterramento ou ficar perto de árvores. Você é uma bateria biológica. Quando sente fome, é o sistema digestivo eliminando resíduos e toxinas do corpo. É importante jejuar, pois após dois dias o corpo produz células-tronco para se regenerar." (PE5)

Chart 1: Representative excerpts from each category

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APRENDIZAGEM BASEADAS EM PROJETOS: ENSINO DE ÁCIDO-BASE, ESTEQUIOMETRIA E LIGAÇÕES QUÍMICAS ATRAVÉS DO PROJETO SÍNTESE DO COTIDIANO.

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Palavras Chave:*PIBID,Funções Inorgânicas,Estequiometria,Ligações Químicas,Práticas Experimentais.*

Highlights

Education is still traditional,The quest for new active learning methodologies, New Chemistry education models,Contextualization with cleaning products,Active participation of students.

Resumo/Abstract

O ensino de Química enfrenta desafios de superar modelos educacionais tradicionais e ultrapassados. Embora seja uma ciência fundamental para áreas como medicina e indústria, a educação Química ainda é dominada por um modelo tradicional centrado na memorização de fórmulas, regras e nomenclaturas, geralmente sem conexão com a realidade social dos alunos. No contexto da turma do 1° ano do curso técnico em Edificações do Instituto Federal de Alagoas - Campus Maceió, verificou-se que muitos alunos observavam a Química com conceitos puramente abstratos. Desta forma, este trabalho objetivou engajar os estudantes na investigação de problemas químicos do cotidiano, permitindo que eles desenvolvam conhecimentos e habilidades essenciais por meio de um processo de construção ativa em aulas experimentais. Para tal ação, os bolsistas do PIBID intervieram, com suporte da professora supervisora, introduzindo práticas experimentais com situações do cotidiano, p.e. 1) Estudando estequiometria através da produção de sabão; 2) Estudando ligações químicas através da produção de desinfetante e 3) Estudando ácidos e bases através da produção de multiuso. A análise dos relatos dos discentes, p.e. “executar o procedimento me permitiu perceber como cálculos de mols, massa molar, proporções e propriedades das substâncias, realmente se aplicam na prática” (A2), revelou que as práticas experimentais favoreceram a apropriação conceitual, funcional e integrada dos conteúdos químicos, frequentemente abordados de forma abstrata no ensino médio. A intervenção demonstrou que a experimentação investigativa é uma alternativa eficaz ao ensino tradicional, ao produzir os produtos de limpeza os discentes puderam visualizar a Química na prática e começar a visualizar como uma ciência verdadeiramente aplicada.



Produto gerado em uma das aulas experimental

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A Química nos livros didáticos de projetos integradores de Ciências da Natureza do PNLD 2026

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Palavras Chave:*Projetos integradores,Livros didáticos,Ensino de química,PNLD 2026*

Highlights

O estudo visa analisar como os conhecimentos de Química são abordados nos livros de projetos integradores de Ciências da Natureza aprovados no PNLD 2026.

Resumo/Abstract

Em 2019, a proposta do Programa Nacional do Livro Didático (PNLD) incluiu os livros didáticos dos projetos integradores, medida implementada a partir de 20201. Os projetos integradores propostos pela Base Nacional Comum Curricular (BNCC) foram incorporados à Educação Básica nos itinerários formativos, com o objetivo de articular temas do cotidiano e integrar diferentes campos do conhecimento. Assim, o objetivo deste estudo é analisar como a Química é articulada nos projetos propostos nos livros didáticos de projetos integradores de Ciências da Natureza para o Ensino Médio, aprovados no PNLD 2026. A pesquisa adotou uma abordagem metodológica qualitativa, baseada na análise documental desses materiais por meio da análise de conteúdo[2]. Cada livro analisado contém seis projetos integradores, com temas relacionados às três principais áreas das Ciências da Natureza. No entanto, apenas dois estão relacionados diretamente a conteúdos de Química. De modo geral, os projetos seguem uma estrutura pedagógica que começa com a problematização de situações, para contextualizar os conteúdos escolares, estabelecer conexões significativas com a realidade dos estudantes e auxiliar na compreensão. A análise dos livros didáticos mostrou que os conteúdos de química são majoritariamente associados a questões ambientais, sociais e tecnológicas, facilitando a compreensão dos conceitos científicos. Todavia, a proposta dos projetos integradores de Química no PNLD 2026 prioriza uma aprendizagem na prática; observa-se uma limitação significativa quanto ao aprofundamento conceitual. Os assuntos são abordados de forma simplificada que não considera a complexidade conceitual. Conclui-se que os projetos integradores devem incorporar maior aprofundamento conceitual para promover uma aprendizagem efetiva.

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Coleção	Projeto Integrador de Química
Ciências da Natureza em Movimento	Plásticos: por que Substituí-los?;
	Água da Chuva: É Possível Utilizá-la?;
Moderna em Projetos: Ciências da Natureza	Consumo Consciente e Noções de Educação Financeira;
	Questões ambientais: infografando e propondo soluções
Intereação Ciências da Natureza e suas Tecnologias	Energia Sustentável: o Futuro Deve Ser Agora!;
	Saneamento Básico: uma Questão Socioambiental;

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Assimetria de gênero nos livros didáticos de Química aprovados no PNLD-2026.

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Palavras Chave:*Women in science,Gender asymmetry,Science communication*

Highlights

An analysis of how women scientists are represented in chemistry textbooks approved by PNLD 2026.

Resumo/Abstract

Mulheres cientistas têm conquistado maior protagonismo nos últimos anos, porém muitas pesquisadoras e suas contribuições ainda permanecem invisibilizadas e desvalorizadas, aumentando a assimetria de gênero principalmente nas ciências exatas[1] .Uma das estratégias para contornar essa realidade é ampliar a divulgação dessas contribuições na educação básica, sobretudo por meio dos livros didáticos, principal recurso pedagógico utilizado por estudantes da rede pública brasileira. Esses materiais são avaliados e distribuídos pelo Programa Nacional do Livro e do Material Didático (PNLD). O objetivo deste trabalho é avaliar como as mulheres cientistas e suas contribuições estão inseridas nos livros didáticos de Química aprovados para escolha do PNLD-2026. A pesquisa foi organizada a partir da avaliação de nove livros didáticos, com análise de caráter qualitativo e coleta do tipo documental, observando as citações de cientistas presentes no corpo do texto, em seções especiais e em boxes explicativos. Os resultados da pesquisa mostram que estes livros didáticos apresentam poucas citações sobre cientistas mulheres e seus trabalhos, além de grande discrepância na quantidade de referências entre as obras analisadas. O livro Moderna Plus destacou-se com 36 citações, o que pode estar relacionado ao fato de ser escrito por duas mulheres. Marie Curie foi a cientista mais mencionada, possivelmente devido à relevância histórica de suas contribuições e ao fato de ser a única mulher a receber dois prêmios Nobel. Embora haja avanços pontuais, a presença feminina ainda é limitada e marcada por desigualdades, quando citadas, geralmente são de forma superficial e em espaços marginais. Dessa forma, é necessário um trabalho de conscientização com os autores e elaboração de políticas públicas de modo que se possa garantir maior destaque às mulheres cientistas e suas contribuições.

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CCA, IQ-UNESP, PROEC-UNESP

Atividades Experimentais no Ensino Médio: Contribuições do Projeto De Olho na Química no Piauí

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Palavras Chave:*Química Experimental,Experimentação Investigativa,Ensino de Química*

Highlights

Experimentação investigativa no ensino médio.
Divulgação Científica no sertão piauiense.
Experimentação com materiais de baixo custo.

Resumo/Abstract

A Química ainda é percebida por muitos estudantes do ensino médio como uma disciplina abstrata e desafiadora.[1],[2]Com o intuito de minimizar essa dificuldade, o projeto de extensão “De Olho na Química”, vinculado ao curso de Química da Universidade Federal do Vale do São Francisco (UNIVASF), busca aproximar o ensino da Química da realidade dos alunos por meio da experimentação. Criado em 2019, o projeto buscou desenvolver de atividades práticas contextualizadas, contribuindo para um aprendizado mais acessível e significativo. O objetivo deste trabalho foi desenvolver atividades experimentais em escolas de ensino médio da região de São Raimundo Nonato – PI, com a finalidade de tornar o ensino de Química mais concreto, estimular a participação ativa dos estudantes e divulgar o curso de Química da UNIVASF. As ações foram realizadas entre setembro e novembro de 2025, em 4 escolas públicas dos municípios de Fartura do Piauí, São Braz do Piauí, São Raimundo Nonato e Várzea Branca. Foram desenvolvidos experimentos de baixo custo, abordando ácidos e bases, evidências de reações químicas, condutividade elétrica, reações redox, medidas de pH, além da discussão de substâncias presentes no cotidiano. As atividades foram planejadas e executadas por professores e graduandos da UNIVASF, respeitando as condições de infraestrutura. Os alunos foram incentivados a adotar uma postura investigativa, por meio da formulação de hipóteses, observação dos fenômenos e discussão coletiva dos resultados. Apesar das limitações estruturais, verificou-se elevado interesse, curiosidade e engajamento por parte dos estudantes. Ao longo de sua trajetória, o projeto De Olho na Química já promoveu mais de 40 eventos presenciais. Os resultados obtidos evidenciam que a experimentação constitui uma estratégia pedagógica eficaz para promover uma aprendizagem mais interativa e motivadora, reforçando o papel da extensão universitária na democratização do conhecimento e no fortalecimento da educação científica.

Agradecimentos/Acknowledgments

UNIVASF, FAPEPI, INSTITUTO SUA CIÊNCIA

A visita da cientista franco-polonesa Marie Curie ao Estado de São Paulo em 1926

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Palavras Chave:*Mulheres na Ciência,Sociedade de Química de São Paulo,Instituições Científicas,Radioatividade*

Highlights

Marie Curie's visit to São Paulo in 1926, highlighting locations, institutions, activities and demonstrates its potential for teaching Chemistry, the history of science, and female leadership

Resumo/Abstract

Em 1926, a cientista Marie Curie esteve no Brasil, cumprindo uma extensa agenda de atividades no Rio de Janeiro, São Paulo e Minas Gerais. Este trabalho identifica os compromissos cumpridos por Marie no Estado de São Paulo, evidenciando as potencialidades desse evento histórico para o ensino de Química. A pesquisa documental teve como corpus notícias de periódicos brasileiros de 1926 sobre Marie Curie em cidades paulistas. A partir dessas fontes, sistematizamos os locais, personagens e atividades envolvidos na agenda cumprida por ela. A cientista esteve em São Paulo de 13 a 15 de agosto e os resultados destacam as homenagens recebidas por Curie em associações científicas, como a Faculdade de Medicina e Cirurgia, a Sociedade de Química de São Paulo, a Sociedade de Farmácia e Química e a Sociedade de Biologia e Higiene. A programação incluiu uma conferência sobre os fundamentos da radioatividade na Faculdade de Medicina e as visitas a instituições de pesquisa, como o Instituto Butantan e a Estação Biológica do Alto da Serra, e às fontes termais de Águas de Lindóia, revelando o papel das redes científicas e a difusão de conhecimentos químicos emergentes no início do século XX. A análise desse episódio histórico oferece possibilidades educativas ao articular conceitos de radioatividade, história da ciência e contexto social da produção do conhecimento. A incorporação desses acontecimentos em atividades de ensino pode favorecer a compreensão da ciência como uma prática coletiva e institucionalizada, além de contribuir para a contextualização histórica de conceitos químicos. Ao evidenciar a trajetória e o reconhecimento científico de Marie Curie em espaços acadêmicos brasileiros, a abordagem também favorece reflexões sobre a presença e o protagonismo de mulheres na ciência, ampliando referências históricas que podem estimular a participação feminina nas áreas científicas e fortalecer perspectivas educacionais voltada à equidade e à valorização da diversidade na ciência.

Agradecimentos/Acknowledgments

Ao Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq - Processos: 409697/2023-0; 315155/2023-0; 440721/2024-5.

Awakening Potential: Teaching and Research for Students with High Abilities in the DF

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Palavras Chave:*Data Sciences,Quantum Technologies,Theoretical and Computational Chemistry,Practical Laboratory*

Highlights

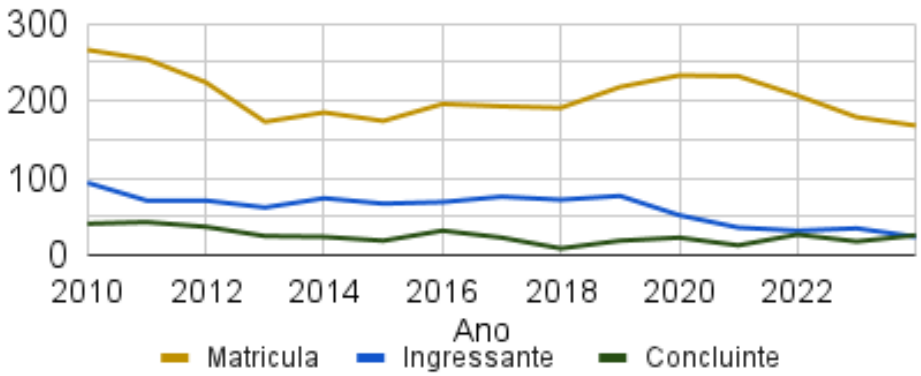
Highlight the importance of awakening scientific vocation and fostering talent development through the participation of gifted high school students in extension projects at Brasília University.

Resumo/Abstract

This work is the result of the Extension Project: “Theoretical and Computational Chemistry in Basic Education: Learning by Doing” which aims to integrate University-Society through assistance to High School students with High Abilities/Giftedness (AH/SD). Despite pioneering advances, Brasília still faces gaps in specialized educational services. This project provides students with academic experiences and knowledge of theoretical and computational chemistry for life.

The method consists of some steps such as: carrying out bibliographical surveys on social issues of interest to students. Next, computational chemistry techniques are applied to construct and optimize molecular structures related to the themes, using the MMFF94 force field and the AM1 semi-empirical method, to then calculate physicochemical descriptors.

The results include the promotion of scientific thinking through accessible computational chemistry activities and critical reflection on the role of the extension student as a protagonist in the construction of knowledge both at the university level and in the external community context. The approach strengthened student protagonism, culminating in nine themes on social issues of interest to students. One of the biggest impacts of this project is the entry of participants into undergraduate Chemistry courses. This entry is significant, considering the downward trend in enrollment in courses in the area in recent years (Figure), observed through statistical data from the Higher Education Census.
The project proves to be an effective strategy to enrich the training of students with AH/DS, offering a challenging and investigative environment that meets their singularities and promotes inclusion. This initiative not only stimulated new scientific vocations, but also transformed knowledge and technology into science made for people who together can transform knowledge into sovereignty.



Statistical data from Higher Education Census

Agradecimentos/Acknowledgments

The authors gratefully acknowledge the Brasília University, particularly the Extension Department, for financial support, and the Computational Chemistry Laboratory of the Institute of Chemistry for the infrastructure and support provided.

Calorímetro de Baixo Custo para Experimentação no Ensino de Química Utilizando as Plataformas ESP8266 e ThingSpeak

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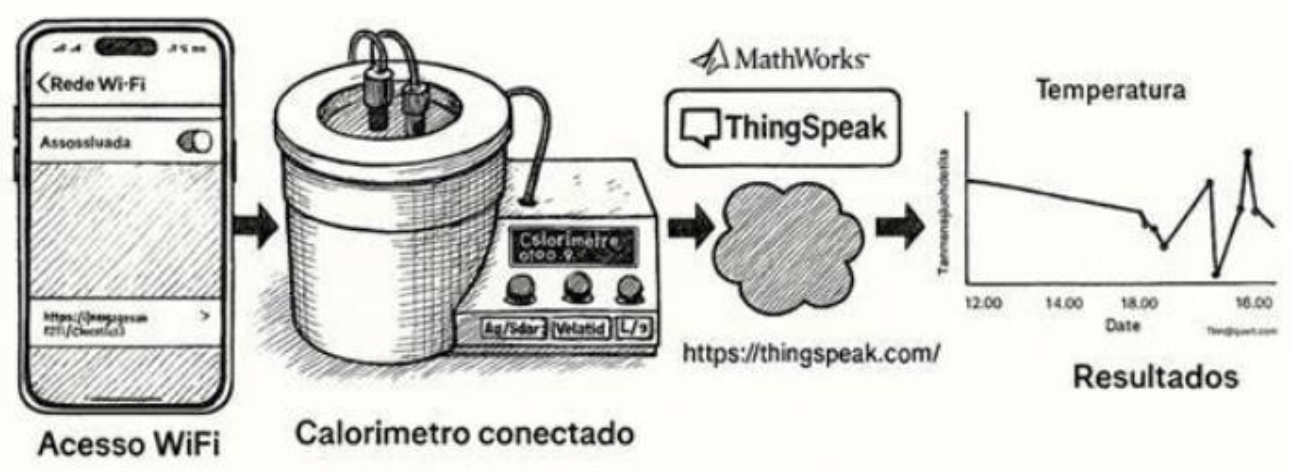
Palavras Chave:*Automação, Conectividade, Aprendizado, Ensino público.*

Highlights

O calorímetro proposto favorece a compreensão de conceitos físico-químicos, estimula a interdisciplinaridade e a inovação pedagógica, tornando o ensino mais dinâmico e inclusivo.

Resumo/Abstract

A experimentação desempenha papel central no ensino de Ciências, e a adoção de práticas remotas tem se mostrado uma alternativa eficaz para ampliar o acesso dos estudantes a atividades laboratoriais. Nesse contexto, apresenta-se o desenvolvimento final de um calorímetro de baixo custo integrado ao microcontrolador ESP8266, projetado para operar tanto localmente quanto de forma remota. A conexão do dispositivo à internet ocorre via roteamento por smartphone, permitindo que todas as etapas de entrada, saída e armazenamento de dados sejam realizadas pela plataforma ThingSpeak. As medições de temperatura em função do tempo são automaticamente convertidas em planilhas e gráficos, facilitando a análise pelos alunos. O protótipo possibilita a execução de experimentos clássicos de termoquímica, como determinação da capacidade térmica do calorímetro, entalpia de neutralização ácido base e entalpia de dissociação. Testes preliminares de usabilidade demonstraram boa concordância entre as leituras do termopar e de um termômetro de bulbo de mercúrio, apresentando perfis térmicos equivalentes. A capacidade térmica obtida para o protótipo (19,39 cal/°C) foi comparada à de um calorímetro educacional comercial (24,48 cal/°C), ambos situados na faixa recomendada pela literatura para minimizar interferências no balanço energético (15 a 25 cal/°C). Os resultados evidenciam que o sistema apresenta desempenho adequado para fins didáticos, aliando baixo custo, acessibilidade e integração digital. A proposta contribui para a inovação no ensino de Química ao favorecer práticas experimentais contextualizadas, interdisciplinares e alinhadas às demandas contemporâneas de aprendizagem mediada por tecnologias.



Representação metodológica do calorímetro educacional de baixo custo integrado à plataforma ESP8266.

Agradecimentos/Acknowledgments

Ao IFSP – Campus Campinas pela infraestrutura para execução do projeto e financiamento através de bolsa PIBIFSP. A Inova/PRP pelo aporte financeiro através dos editais de fomento aprovados.

CHEMOPOLY: A INDÚSTRIA QUÍMICA COMO EIXO PARA O ENSINO DE QUÍMICA INORGÂNICA EM UM JOGO DIDÁTICO

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Palavras Chave:*Tabuleiro,Propriedade Periódica,Química Inorgânica,Indústria Química,Aprendizagem Lúdica*

Highlights

Board game based on the Periodic Table connects inorganic chemistry concepts to industrial applications, promoting active, contextualized, and meaningful learning through gameplay.

Resumo/Abstract

O CHEMOPOLY é um jogo didático de tabuleiro inspirado na dinâmica do jogo comercial Monopoly, desenvolvido para a consolidação de conteúdos de Química Inorgânica no Ensino Médio. O tabuleiro é estruturado de modo que cada conjunto de cores represente um grupo da Tabela Periódica, associando elementos químicos às suas principais aplicações tecnológicas e industriais. Ao longo das quatro fileiras distribuem-se indústrias, refinarias e usinas relacionadas aos respectivos elementos, como a fábrica de baterias de lítio posicionada junto ao grupo dos metais alcalinos, favorecendo a aprendizagem por correlação entre propriedades químicas e usos cotidianos, conforme ilustrado na Figura 1. O jogo inclui cartas especiais denominadas Fundo de Pesquisa e Reação Inesperada, que substituem, respectivamente, as tradicionais cartas de cofre e sorte. As cartas de Fundo de Pesquisa apresentam informações conceituais sobre elementos e famílias químicas, enquanto as cartas de Reação Inesperada trazem questões objetivas que resultam em ganhos ou perdas de recursos conforme as respostas dos jogadores. A moeda do jogo, denominada mols, é utilizada para a aquisição de laboratórios e registro de patentes, correspondentes aos terrenos e casas do jogo original. Quando um jogador cai em um laboratório pertencente a outro, paga-se um valor referente à “pesquisa científica”, que aumenta de acordo com o número de patentes e indústrias instaladas. Essa dinâmica integra conteúdos de Química, tecnologia e economia, estimulando o raciocínio estratégico, a tomada de decisões e a aprendizagem ativa. O CHEMOPOLY contribui para a compreensão da organização da Tabela Periódica, das propriedades dos elementos e de suas aplicações no contexto real, configurando-se como um recurso pedagógico inovador e contextualizado para o ensino de Química.



Figura 1. Tabuleiro do jogo e suas cartas.

Agradecimentos/Acknowledgments

IFCE – Campus Aracati

PIBID – Sub-projeto Química – IFCE – campus Aracati

CAPES

CHON – The Chemist's Domino

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Palavras Chave:*Organic Chemistry,Interactive Game,Chemical Bonds,and Dominoes,Dominoes*

Highlights

CHON – Uses domino logic to model bonds between C, H, O, and N, enabling molecular construction according to valence rules and promoting active learning in Organic Chemistry.

Resumo/Abstract

CHON – The Chemist's Domino consists of the proposal of an educational game developed as a didactic resource to support the teaching of introductory concepts in Organic Chemistry. The proposal aims to promote the understanding and visualization of chemical bonding among the main elements that constitute organic molecules: carbon (C), hydrogen (H), oxygen (O), and nitrogen (N). Inspired by the structure of the traditional domino game, the numbers are replaced by chemical symbols and their respective valences, allowing the tiles to be connected according to the possibilities for covalent bond formation. The game dynamics are based on the equal distribution of tiles among the participants and on the need to connect them according to the compatibility between the represented valences. When no valid move is possible, the participant discards a tile and passes the turn. As connections are made, players may form stable molecular structures, and the complete formation of these structures allows the collection of the corresponding tiles. At the end of the game, the winner is the participant who accumulates the largest number of tiles. This work presents the conception and planning of the game as a pedagogical proposal and does not yet include results from classroom implementation. However, the process of developing the material constituted an important formative experience for the students involved in the project, who participated in conceptual discussions about valence, chemical bonding, and molecular representation, as well as in the process of translating these concepts into a playful and accessible format. This stage contributed to the development of skills related to the organization of chemical knowledge, creativity in the production of teaching resources, and reflection on teaching strategies aimed at promoting greater engagement and conceptual understanding of Chemistry content.



Application of the CHON game in a chemistry class at IFCE – Aracati.

Agradecimentos/Acknowledgments

IFCE – Campus Aracati

PIBID – Sub-projeto Química – IFCE – campus Aracati

LEMA – Laboratório de Ensino Maker do Aracati

CAPES

Conceptions, Proposals, and Limitations of Chemistry Undergraduates Regarding the Inclusion of Diversity and Interculturality in Teaching Practice

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Palavras Chave:*Teacher training,Science education,Cultural diversity,Interculturality,Teaching practice*

Highlights

Valuing diversity in chemistry education.

Integrating traditional knowledge.

Weaknesses in teacher training for inclusive practices.

Resumo/Abstract

Diversity is a human condition that should be valued and seen as a richness. In the educational context, interculturality emerges as an essential approach to promote a democratic, inclusive, and just society. Thus, this study analyzed the expectations, proposals, and perceptions of undergraduate students in the Chemistry Licentiate program at the Federal University of Maranhão regarding the incorporation of diversity and interculturality into their future teaching practice. The research, using a qualitative approach and being an exploratory case study, was conducted through semi-structured interviews applied to seven undergraduate students, whose data were organized into thematic categories using Content Analysis, forming analytical blocks that constitute the systemic network. The results show that the participants recognize the importance of valuing cultural diversity in the teaching of Science and Chemistry, highlighting the need for the integration of traditional, indigenous, and Afro-Brazilian knowledge into scientific content as a relevant and contextualized pedagogical strategy. A vision of humanized and welcoming teaching, based on empathy, dialogue, and the collective construction of knowledge, also emerged. However, the study reveals weaknesses related to the practical application of these approaches, mainly associated with deficiencies in training and the absence of theoretical and methodological frameworks during initial teacher training. The statements indicate that these gaps generate insecurity and limit the implementation of inclusive practices, reinforcing the need for teacher training that systematically and transversally addresses diversity, interculturality, and inclusive education. It is concluded that strengthening professional and curricular knowledge is fundamental to supporting critical, culturally contextualized, and socially committed pedagogical practices in the teaching of Science and Chemistry.

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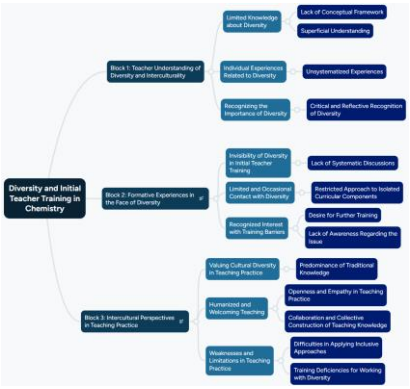


Figure 1: Systemic network for analyzing student responses regarding diversity and teaching knowledg

Agradecimentos/Acknowledgments

We thank the Federal University of Maranhão (UFMA), the Research Group in Science and Chemistry Education (GPECNQ+), and FAPEMA for their institutional and scientific support in the development of this study.

Contribuições dos kits da Experimentoteca disponíveis no Centro de Ciências de Araraquara para educação básica da região de Araraquara

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Palavras Chave:*Experimentoteca-Ensino de Ciências-Centro de Ciências*

Highlights

Realizou-se uma análise do número de kits experimentais da Experimentoteca distribuídos na região de Araraquara pelo Centro de Ciências e do número de alunos beneficiados por eles.

Resumo/Abstract

Atividades experimentais são fundamentais para o processo de ensino aprendizagem, vinculam a teoria com a prática e despertam o interesse dos alunos, no entanto, os professores enfrentam obstáculos para aplicar atividades experimentais devido à falta de estrutura. O censo escolar de 2024 mostra que no estado de São Paulo 31% das escolas de ensino fundamental e 37% de ensino médio possuem laboratório de ciências. A Experimentoteca é um conjunto de kits experimentais itinerantes que são disponibilizados aos usuários mediante empréstimos gratuitos; ela foi desenvolvida no Centro de Divulgação Científica e Cultural (CDCC) da USP de São Carlos. O Centro de Ciências de Araraquara (CCA) possui 40 kits que circulam pelas escolas da região, permitindo que elas levem experimentos até os seus alunos. Neste trabalho analisaram-se registros de empréstimos dos kits de 1999 até 2025, no entanto, o CCA trabalha com os kits desde 1992 quando se instalava na escola ETEC Profª Anna de Oliveira Ferraz, sendo 1999 o ano em que se iniciaram as atividades no espaço atual. A pesquisa mostrou que o CCA distribuiu 140 kits, alcançando cerca de 8500 alunos no ano de 2001. Números significativos de empréstimos se mantêm até 2005 atingindo entre 3000 e 7000 alunos, o segundo ano de maior alcance foi em 2000, com 7600 alunos beneficiados e 131 empréstimos. De 2005 a 2014, houve uma queda considerável com valores inferiores de 60 kits emprestados. No período de 2015 a 2022 não se tem registros e acredita-se que o motivo seja a falta de controle desses empréstimos, o período de pandemia de Covid-19 e a transição de diretores. O retorno, em 2023, é marcado por baixos números de empréstimos e se estende até 2025. Visto que os kits contribuem para a acessibilidade da ciência experimental, o projeto visa a ampla divulgação para que eles tenham maior alcance, além da manutenção e preservação deles. Referência: Censo escolar 2024: https://anuario.todospelaeducacao.org.br/2025/estados-sp.htm

Agradecimentos/Acknowledgments

Centro de Ciências de Araraquara (CCA)

Cultivo do melão Gaúcho: desenvolvimento de uma Unidade Temática fundamentada na abordagem CTS para o ensino de Química

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Palavras Chave:*Ensino de Química, Cultivo do melão Gaúcho, Unidade Temática, CTS.,Ensino de Química,Cultivo do melão Gaúcho,Unidade Temática,CTS*

Highlights

High school students conducted soil analysis experiments and developed materials to enable the replacement of newspaper leaves in cultivating the Gaúcho melon. Thematic unit based on the STS approach.

Resumo/Abstract

Neste trabalho é relatado o desenvolvimento e a aplicação de uma Unidade Temática (UT) fundamentada nas relações entre Ciência, Tecnologia e Sociedade (CTS), compreendidas como uma abordagem que visa promover atitudes e valores cidadãos por meio da articulação entre conhecimentos científicos, tecnológicos e o contexto social. O estudo foi desenvolvido no âmbito do PROFQUI/UFRGS e aplicado em uma escola pública do município de Nova Santa Rita/RS, reconhecido como um dos principais produtores de melão do estado. A problemática emergiu da própria comunidade escolar, composta em parte por agricultores, que relataram dificuldades no uso de folhas de jornal para a proteção do melão Gaúcho durante o crescimento dos frutos, em função da redução da circulação de jornais impressos e do consequente aumento do custo de produção. A partir desse contexto, foi elaborada uma UT que abordou os conceitos de elementos químicos, tabela periódica, íons, acidez e pH, articulados ao cultivo do melão. Por intermédio do auxílio da prefeitura municipal, agrônomos da Empresa de Assistência Técnica e Extensão Rural do Rio Grande do Sul (Emater) e de um produtor rural foi construída uma lavoura experimental na escola para o cultivo do melão Gaúcho. A UT teve duração de 16 encontros de três horas, com a participação de 16 estudantes no contraturno. As atividades incluíram a manutenção da lavoura, análises de solo e o desenvolvimento de materiais alternativos às folhas de jornal para proteção dos frutos. Os resultados indicam a compreensão dos conceitos químicos relacionados ao cuidado do solo e as substâncias necessárias para tal. Entre os materiais testados experimentalmente, destacou-se um produto obtido a partir de resíduos orgânicos, especialmente cascas de ovos, que se mostrou uma alternativa viável às folhas de jornal. Conclui-se que o ensino de Química foi fortalecido pela contextualização e pela participação ativa dos estudantes no desenvolvimento de uma tecnologia socialmente relevante.



Graphical Abstract

Agradecimentos/Acknowledgments

À comunidade da Escola Estadual de Educação Básica Santa Rita, aos funcionários da prefeitura municipal de Nova Santa Rita/RS, aos agrônomos da EMATER/RS e do produtor rural parceiro do projeto.

Da Universidade ao Território: O Programa 1000 Futuros Cientistas e a Construção da Cultura Científica na 22ª SNCT

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Palavras Chave:*Educação Científica,Extensão Universitária,Divulgação Científica,Sustentabilidade,Ensino de Química*

Highlights

O VII Dia com Ciência integrou ensino, pesquisa e extensão na 22ª SNCT, fortalecendo a formação docente e discente e a promoção de uma educação científica comprometida com os desafios socioambientais.

Resumo/Abstract

A 22ª Semana Nacional de Ciência e Tecnologia teve como tema central “Planeta Água: Cultura Oceânica para Enfrentar as Mudanças Climáticas no Meu Território”, evidenciando a centralidade da educação científica frente aos desafios socioambientais. Nesse contexto, o programa de extensão 1000 Futuros Cientistas, vinculado à UFMG, desenvolveu o evento VII Dia com Ciência, com apoio do CNPq e da FAPEMIG, com o objetivo de incentivar a realização de novas ações similares e promover a formação de discentes articulada com a extensão, a pesquisa e a sociedade, contribuindo para a formação docente e a promoção de uma educação científica comprometida com os desafios territoriais e ambientais contemporâneos, em consonância com os objetivos da SNCT e com os debates da área de Ensino de Química. O VII Dia com Ciência foi estruturado a partir de um evento central e de ações satélites, ampliando o alcance territorial das atividades de divulgação científica e formação docente. O evento central, o II Professor Protagonista no Ensino de Química – MG (PEQUI-MG), realizado em 16 e 17 de outubro de 2025, reuniu mais de 100 participantes, entre licenciandos e professores da educação básica, e contou com a submissão de 15 trabalhos, além de palestras, oficinas, workshops e atividades experimentais, abordando temas como economia circular, valorização dos saberes tradicionais, sustentabilidade e mudanças climáticas, articulados ao ensino de Química. As ações satélites incluíram iniciativas como o UFMG nas Ruas, o EcoParque 2025 e a ação Experimentando Ciência no DQ, promovendo oficinas, atividades experimentais e vivências em espaços públicos, escolas e laboratórios universitários. A análise das ações evidenciou o fortalecimento da cultura científica, maior engajamento do público e ampliação da percepção da Química como conhecimento contextualizado e socialmente relevante, além de maior segurança dos professores para incorporar práticas experimentais e abordagens interdisciplinares.

Agradecimentos/Acknowledgments

CNPQ, FAPEMIG, DQUFMG, INCT MIDAS; INCT UREASE, INCT SUBSTÂNCIAS PSICOATIVAS, PROEX, PPGIT. PPGQ

Descarte de pilhas como temática socioambiental no Ensino de Química: um projeto de extensão com abordagem experimental e formativa

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Palavras Chave:*Ensino de Química,Extensão Universitária,Educação Ambiental,cccc*

Highlights

Este trabalho envolve ações extensionistas que buscam demonstrar a importância da Química na formação de cidadãos críticos e preocupados com o meio ambiente através da temática descarte de pilhas.

Resumo/Abstract

Este trabalho descreve um projeto de extensão universitária em fase inicial, desenvolvido ao longo de dois meses junto a estudantes de Engenharia Química, que participaram do planejamento e da execução das atividades. Uma das ações extensionistas consistiu na visita de uma turma com 21 alunos da 2ª série do Ensino Médio, provenientes de uma escola de educação básica, à universidade. Nesse encontro, iniciou-se a coleta de pilhas usadas, com o objetivo de recuperar materiais que possam ser reutilizados em atividades experimentais. Durante a visita, também foram discutidos os impactos ambientais associados ao descarte inadequado de pilhas, relacionando esse tema a conceitos químicos e buscando promover a conscientização por meio da articulação entre educação ambiental, ensino experimental e formação crítica.

A partir desse encontro, foi possível discutir com os estudantes da educação básica alguns princípios da Química Verde, estabelecendo relações com debates sobre ciência, tecnologia, sociedade e meio ambiente. Essa abordagem pode contribuir para a promoção de uma educação ambiental crítica, voltada para a formação cidadã (Sandri e Filho, 2019).

Além disso, a atividade teve relevância formativa para os estudantes de Engenharia Química, que participaram ativamente do processo educativo, contribuindo para a construção da aprendizagem relacionada a conceitos de eletroquímica. O contato com os fundamentos da Química Verde também se mostra importante na formação desses futuros profissionais, considerando sua relevância para a prática da Engenharia Química (Patre at. al., 2023).

Como perspectivas futuras, prevê-se a construção de kits para experimentos com material recolhido que serão doados às escolas.

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DESENHO UNIVERSAL PARA A APRENDIZAGEM NO ENSINO DE QUÍMICA PARA ESTUDANTES COM DEFICIÊNCIA VISUAL: REVISÃO DE ESCOPO

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Palavras Chave:*Desenho Universal para a Aprendizagem,Educação Inclusiva,Deficiência Visual,Ensino de Química,Ensino Médio.*

Highlights

How inclusive is Chemistry education? This scoping review shows that Universal Design for Learning has potential for visually impaired students but reveals gaps in secondary education research.

Resumo/Abstract

A inclusão de estudantes com deficiência visual no ensino de Química exige abordagens pedagógicas que considerem a diversidade de modos de aprendizagem. O Desenho Universal para a Aprendizagem (DUA) destaca-se como um referencial promissor ao propor múltiplas formas de ação. Entretanto, sua aplicação no ensino de Ciências, especialmente da Química, direcionada a estudantes com deficiência visual, ainda se apresenta de forma fragmentada na literatura. Este estudo teve como objetivo mapear e caracterizar evidências científicas sobre metodologias fundamentadas no DUA aplicadas ao ensino de Ciências, com ênfase no ensino de Química, destinadas a estudantes do ensino médio com deficiência visual. Trata-se de uma revisão de escopo conduzida conforme a metodologia do Joanna Briggs Institute (JBI) e reportada segundo as diretrizes do PRISMA-ScR. A busca foi realizada nas bases ERIC, Scopus, Web of Science, SciELO e Google Scholar, contemplando estudos publicados entre 2021 e 2025, nos idiomas português, inglês e espanhol. Utilizaram-se descritores combinados por operadores booleanos*AND*e*OR*, incluindo desenho universal para a aprendizagem, educação inclusiva, deficiência visual, ensino de ciências e ensino médio. Após a aplicação dos critérios de inclusão e exclusão, os estudos foram analisados quanto ao tipo de evidência, público-alvo, nível de ensino e estratégias pedagógicas. Os resultados indicam predominância de revisões sistemáticas e estudos aplicados, voltados à educação básica e ao ensino superior. Observa-se escassez de investigações empíricas direcionadas ao ensino médio e à deficiência visual, bem como lacunas na aplicação do DUA. As evidências apontam que estratégias fundamentadas no DUA favorecem o acesso aos conteúdos, o engajamento e a participação dos estudantes. Conclui-se que há necessidade de ampliar pesquisas empíricas no ensino médio, ensino de Química para estudantes com deficiência visual.

Agradecimentos/Acknowledgments

Esta pesquisa tem apoio da UNESPAR/Campus União da Vitória e da Secretaria de Estado da Ciência, Tecnologia e Ensino Superior do Paraná (SETI).

Desenvolvimento de modelos 3D para o ensino de biomoléculas e biotecnologia

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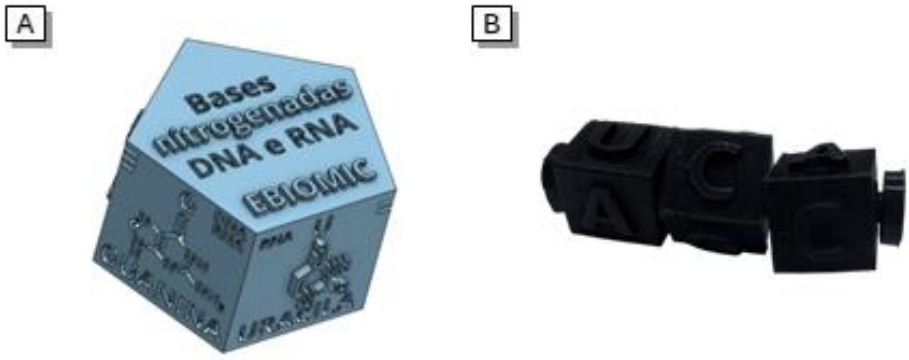
Palavras Chave:*Impressão 3D,Projeto maker,Multimodalidade,Macromoléculas,Microrganismos*

Highlights

Desenvolvimento de modelos 3D didáticos para kits de biomoléculas e de microrganismos. Pluralismo estratégico para ensino de ciências.

Resumo/Abstract

O ensino de ciências, sobretudo a química e bioquímica, é marcado por conceitos abstratos e desafios recorrentes na práxis de professores, como carência de infraestrutura e escassez de materiais didáticos adequados. Diante deste cenário, são necessárias estratégias didáticas que articulem os níveis macroscópico, submicroscópico e representacional, favorecendo a apropriação dos conhecimentos científicos pelo estudante no processo de ensino e aprendizagem. Assim, a universidade pode contribuir com a educação escolar, desenvolvendo recursos que ampliem as estratégias no ensino de ciências. Desta forma, o objetivo deste trabalho foi desenvolver kits para a execução de experimentos educativos no ensino de química e bioquímica no ensino médio, em específico, a produção de modelos 3D. Para o desenvolvimento dos modelos, foi realizado um levantamento bibliográfico das concepções alternativas e obstáculos epistemológicos, seguido da análise de modelos tridimensionais didáticos existentes. Como resultado, observou-se poucos modelos didáticos adequados ao ensino de biomoléculas, apresentando limitações quanto ao detalhamento, clareza conceitual e interatividade com planejamento didático intencional, restringindo-se a modelos de encaixe. Diante dessas lacunas, foram desenvolvidos modelos 3D impressos em filamento de ácido polilático (PLA), selecionado pelo baixo custo, resistência e menor impacto ambiental. Entre os modelos projetados, destaca-se para os lipídeos uma micela com ímãs para demonstrar seu caráter anfipático; uma proteína, no formato de "boneca russa", que permite visualizar diferentes níveis estruturais; e para o DNA, além da dupla hélice a inclusão de um prisma representando as bases nitrogenadas e um códon interativo, para auxiliar na relação dos aminoácidos (Figura 1). Assim, os modelos desenvolvidos ampliam a visualização e a compreensão dos conteúdos pelos estudantes, contribuindo para superar dificuldades de aprendizagem no ensino de química e bioquímica.



Modelos tridimensionais: A - Bases nitrogenadas e B - modelo interativo de códons (impresso).

Agradecimentos/Acknowledgments

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Desenvolvimento de um jogo didático para o ensino de Química Verde sob a ótica da abordagem STEAM

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Palavras Chave:*Química Verde, Ensino de Química, Abordagem STEAM, recurso didático,Química Verde, Ensino de Química, Abordagem STEAM, jogo didático,Química Verde, Ensino de Química, Abordagem STEAM, Jogo didático*

Highlights

Green Chemistry applied to science education.

STEAM education.

Integrating STEAM and Green Chemistry.

Green Chemistry for high schools.

Game-based learning applied to science education.

Resumo/Abstract

Historicamente, o ensino de Química no nível médio enfrenta o desafio de superar abordagens tradicionais, muitas vezes restritas à memorização de fórmulas e à fragmentação do conhecimento. Diante desse cenário, torna-se relevante a busca por alternativas pedagógicas que facilitem a ampliação do conhecimento científico e que também promovam um engajamento discente efetivo.
Dessa forma, este trabalho propõe a elaboração de um jogo didático no qual os estudantes possam aprimorar seus conhecimentos de Química Verde sob a ótica STEAM (sigla em inglês para Ciência, Tecnologia, Engenharia, Artes e Matemática), perspectiva essa que tem demonstrado ser uma abordagem relevante no desenvolvimento do pensamento crítico e no fortalecimento da interdisciplinaridade. Ao articular a criatividade com o rigor científico, essa abordagem busca instigar o aluno a questões mais complexas, seguindo os 12 princípios fundamentais da Química Verde.
A estruturação do jogo, com questões baseadas em Química Verde e divididas pelas categorias da abordagem STEAM, fomenta o desenvolvimento de competências em cada área. Nesse sentido, o jogo, voltado para grupos de alunos do Ensino Médio, adota uma mecânica de risco e recompensa aplicado ao ensino de Química Verde que, portanto, percorre-se pelo tabuleiro onde cada casa aciona uma pergunta temática, estimulando continuamente o estudante a tentar desafios maiores, afinal, acertos de questões complexas geram mais recursos. Desse modo, o projeto dedica-se a promover habilidades cognitivas e intelectuais, conectando o aprendizado conceitual à motivação e à interação colaborativa entre os alunos.

Agradecimentos/Acknowledgments

À FAPESP, UNICAMP, Instituto de Química da UNICAMP, co.educa, Canal Futura — Fundação Roberto Marinho, CNPq, CAPES e ao programa Praticar Ciência.

Design thinking aplicado ao ensino de química e seu impacto na divulgação científica enquanto extensão universitária

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Palavras Chave:*Design thinking,Ensino de química,Educação básica,Popularização da ciência*

Highlights

Design-driven communication as a tool to enhance chemistry education through university outreach, increasing engagement, accessibility, and student protagonism in university–school partnership.

Resumo/Abstract

A extensão universitária é um eixo estratégico para a promoção da educação e a democratização do conhecimento produzido na universidade pública, especialmente aliada a práticas de divulgação científica em diálogo com a Educação Básica. Nesse contexto, o Programa 1000 Futuros Cientistas (1000FC) desenvolve ações entre universidade e escola com oficinas, feiras científicas, eventos de popularização da ciência e formação docente, com destaque para iniciativas realizadas durante a Semana Nacional de Ciência e Tecnologia.

O trabalho apresenta um relato de experiência sobre a contribuição do design e da comunicação visual como recursos pedagógicos no ensino e na divulgação da Química, a partir da atuação de graduandos em Artes Visuais vinculados à equipe de comunicação do 1000FC. Fundamentado em princípios do design thinking e em abordagens centradas no protagonismo discente, o desenvolvimento dos materiais busca ir além do apelo estético, estruturando experiências educativas acessíveis e inclusivas, adequadas às diferentes faixas etárias do público atendido.

As ações analisadas envolveram a produção de materiais didáticos, identidades visuais de feiras científicas e apoio a oficinas experimentais e eventos formativos, como o Professor Protagonista no Ensino de Química. A partir da observação das atividades, de registros e de relatos de professores e estudantes da Educação Básica, identifica-se indícios de aumento do engajamento, maior participação nas atividades experimentais e percepção positiva quanto à compreensão dos conteúdos de Química. Professores notam maior segurança em sala e reconhecem o design como elemento facilitador da mediação pedagógica.

Resultados indicam que o design, junto a divulgação científica e extensão universitária contribui para promover ambientes de aprendizagem mais acolhedores e estimulantes, e evidencia o potencial formativo interdisciplinar da extensão e o papel do design como ferramenta pedagógica na educação científica contemporânea.

Agradecimentos/Acknowledgments

À equipe do 1000 Futuros Cientistas pela oportunidade de viver a extensão universitária como uma ferramente de divulgação científica e inserção no mercado.

Didactic Evaluation of Reference and Working Electrodes in Electrochemical Experiments

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Palavras Chave:*Electrodes,Electrochemistry,Reference Electrodes*

Highlights

A didactic evaluation of reference and working electrodes in electrochemical experiments is presented. The influence of pH, electrode type, and cell configuration responses are demonstrated.

Resumo/Abstract

In electrochemical experiments, a three-electrode electrochemical cell is used, consisting of a reference electrode (RE), a working electrode (WE), and a counter electrode (CE). The WE is the electrode under study, the RE has a constant and well-known potential, and the CE completes the circuit. Despite its widespread use, there is limited didactic literature addressing the behavior and practical implementation of different reference electrodes under varied experimental conditions, which makes the learning process in Analytical Chemistry courses more challenging. In this work, cyclic voltammetry experiments were performed using platinum (Pt), gold (Au), and glassy carbon (GCE) working electrodes in a solution containing the redox pair $[Fe(CN)_6]^{4-}/[Fe(CN)_6]^{3-}$ at different pH values. Commercial Ag/AgCl, Hg/HgCl, and Hg/HgO electrodes were employed as reference electrodes. A customized 3D-printed cell cap was developed to minimize interference caused by electrode positioning. The results showed good potential stability of the reference electrodes across three measurements. Among the working electrodes, platinum (Pt) exhibited greater reproducibility than gold (Au) and the glassy carbon electrode (GCE), making it the preferred choice for future analyses. These findings highlight the learning of redox reactions when the peaks of the voltammograms are compared, as well as the application of 3D modeling and printing software, which may assist in the development of other devices, such as the construction of an entire electrochemical cell.

Disseminação do tema “Mulheres na ciência” em turmas da Educação de Jovens e Adultos

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Palavras Chave:*Mulheres na Ciência,,Mulheres na Ciência,EJA,História e Filosofia da Ciência*

Highlights

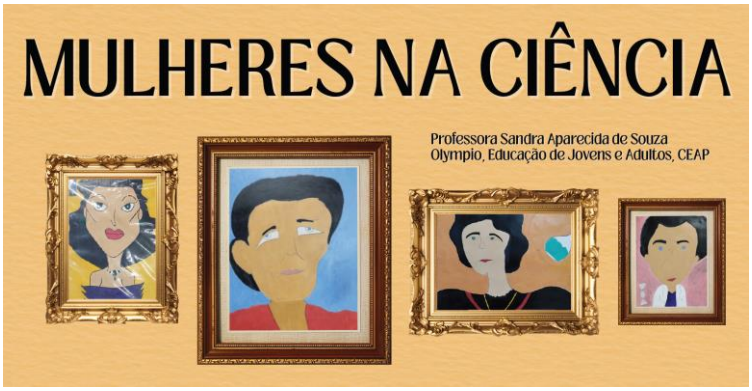
Abordagem e confecção de um livreto com o tema “Mulheres na ciência” em turmas da Educação de Jovens e Adultos (EJA) do Colégio Estadual Américo Pimenta, em Quatis – RJ.

Resumo/Abstract

O tema mulheres na ciência tem ganhado destaque em pesquisas recentes, mas ainda carece de reconhecimento amplo. Um caminho para resgatar e valorizar o protagonismo feminino é por meio da História e Filosofia da Ciência (HFC), que possibilita uma educação crítica ao revelar mulheres esquecidas e desmistificar conceitos tradicionais de ciência. Essa abordagem evidencia as barreiras históricas, sociais e culturais enfrentadas pelas cientistas para conquistar espaço e reconhecimento.[1],[2]

Diante deste problema, esta abordagem foi trabalhada em turmas da Educação de Jovens e Adultos (EJA) do Colégio Estadual Américo Pimenta, em Quatis – RJ, envolvendo 21 alunos (13 mulheres e 8 homens, entre 19 e 70 anos).[3] Foram apresentadas biografias de cientistas das áreas de matemática, física, biologia e química, destacando suas contribuições e descobertas. A partir desse estudo, os alunos foram incentivados a produzir materiais de divulgação sobre as cientistas pesquisadas, onde optaram pela confecção de um livreto, elaborado com textos e imagens caricatas, utilizando ferramentas digitais como o ChatGPT e o Canva. O livreto constitui um produto educacional voltado à disseminação do tema mulheres na ciência, promovendo reflexão crítica e valorização do protagonismo feminino. A experiência demonstrou que, ao integrar HFC e práticas participativas, é possível ampliar o interesse dos estudantes e fortalecer a discussão de gênero na ciência. Conclui-se que essa abordagem contribui positivamente para a educação de mulheres na EJA, estimulando reconhecimento, autoestima e engajamento científico.

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[2] Almerindo, G. I.; et. al;*QNEsc*,**2020**,*42*(4), 344.
[3] Olympio, S. A. S.;*Utilização da história e filosofia da ciência como recurso para mudança de paradigmas de exclusão social: presença das mulheres nas ciências.*Dissertação (Mestrado Profissional em Química) – PROFQUI - UFF, Volta Redonda,**2025**.



Capa do livreto produzido pelas alunas do EJA – Colégio Estadual Américo Pimenta – Quatis / RJ.

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CAPES, FAPERJ, UFF, PROFQUI, Colégio Estadual Américo Pimenta – Quatis/RJ.

Domínios interseccionais do poder e seus atravessamentos para a formação de professores/as de Ciências

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Palavras Chave:*Formação docente,Interseccionalidade,Lei 10.639/03,Licenciatura em Química,Licenciatura em Ciências Biológicas*

Highlights

The intersectional domains of power can contribute to the transgression of a Eurocentric curriculum and support the restructuring of teaching practices in Science education.

Resumo/Abstract

O currículo e a formação de professores/as de Ciências são vilipendiados pelo modelo hegemônico de ser e existir, reverberando no imaginário social compreensão da Ciência como neutra, aproblemática e ahistórica. A reflexão dos domínios interseccionais do poder na formação docente em Ciências pode constituir-se como uma estratégia de ação para os debates sobre as mútuas das relações poder que afetam a sociedade (COLLINS e BILGE, 2020). Com elementos dos pressupostos da Pesquisa Participante, o objetivo deste trabalho foi analisar as contribuições de uma proposição formativa sob um viés das relações interseccionais dos domínios de poder para professores/as de Ciências. A investigação foi desenvolvida ao longo de dezesseis encontros de uma disciplina optativa para licenciandos/as em Química e Ciências Biológicas. A coleta de dados deu-se por meio de registro em áudio e vídeo que posteriormente foram transcritos e analisados à luz dos pressupostos da Análise de Conteúdo (BARDIN, 2021). Em nossos resultados os discursos foram organizados na pré-análise para em seguida agrupar em categorias apriorísticas seguindo as categorias analíticas dos domínios interseccionais do poder: estrutural, disciplinar, hegemônico e interpessoal. Além disso, a partir do tratamento dos resultados e a interpretação, nossos resultados indicam que foi possível operacionalizar os elementos das relações interseccionais visando a formação de professores/as de Ciências para as transformações de suas práticas pedagógicas, assim como os discursos produzidos buscaram romper com a concepção hegemônica de poder.

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A CAPES, o CNPq, o MCTI, o MMulheres, o MIR/UnB, ao PIP e PROLICEN da UFG, a FAPEG e a FUNAPE que possibilitaram o desenvolvimento desta pesquisa.

Educação e Popularização Científica para Redução de Desigualdades: Ações do Núcleo Sudeste da Rede Meninas e Mulheres nas Ciências Exatas

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Palavras Chave:*Mulheres na Ciência,Ensino Médio,ODS 5,Equidade de gênero,Diversidade e inclusão*

Highlights

Encouraging girls to participate in the exact sciences.
Practical and interdisciplinary scientific experiences.
Expanding access to the academic world.

Resumo/Abstract

O Núcleo Sudeste da Rede Meninas e Mulheres nas Ciências Exatas, Computação e Engenharias desenvolveu, em 2025, ações de popularização da Química com o objetivo de promover o protagonismo de meninas do ensino médio e contribuir para a redução das desigualdades de gênero nas STEM. A Química foi adotada como eixo articulador da formação científica, integrando experimentação, reflexão crítica e aproximação com o ambiente universitário. O projeto combinou um ciclo formativo online (oito encontros) e atividades experimentais presenciais na UNESP (Araraquara e Jaboticabal). Os ciclos abordaram gênero e interseccionalidade; violências, sexualidade e ambiente escolar; mulheres, trabalho e carreira acadêmica; mulheres mães cientistas; mulheres negras e indígenas na ciência; e perspectivas contemporâneas para mulheres nas áreas científicas. Esses debates fundamentaram a discussão sobre permanência, pertencimento e identidade científica. As atividades práticas enfatizaram a investigação química como ferramenta de compreensão do mundo material, incluindo oficinas de coleta e análise de impressões digitais, extração de DNA, identificação de substâncias químicas e discussão de métodos analíticos aplicados à perícia criminal. As estudantes visitaram laboratórios de Química e áreas correlatas, tendo contato com rotinas experimentais, instrumentação e processos de pesquisa. Rodas de conversa com docentes, pesquisadoras e uma perita criminal permitiram contextualizar aplicações da Química em diferentes campos profissionais. O acompanhamento foi realizado por meio de relatórios, formulários avaliativos e registros audiovisuais. Os resultados preliminares indicam ampliação do interesse pela Química, maior compreensão do método científico e fortalecimento da autoconfiança acadêmica. A experiência evidencia o papel da experimentação química aliada à discussão crítica de gênero como estratégia efetiva para formação científica inclusiva.

QR Code com acesso a um vídeo elaborado pelas estudantes, registrando as ações realizadas no projeto

Agradecimentos/Acknowledgments

CNPq (Proc. 440721/2024-5) Instituto de Química – UNESP, PROEC-UNESP, UFPR e Paraty Mobility.

Educação Química por investigação em feiras itinerantes: contribuições do 1000 Futuros Cientistas Pelo Mundo

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Palavras Chave:*Educação científica,Extensão universitária,Soberania científica,Ensino de Ciências,Feiras de Ciências*

Highlights

70 basic-education projects presented by students, mentored by teachers & UFMG undergrads. Water quality, recycling and green chemistry grounded in local challenges. Science fair as a learning tool.

Resumo/Abstract

AA aproximação entre universidade, escola e comunidade é estratégica para fortalecer o ensino de Ciências/Química e democratizar o conhecimento científico. Nesse contexto, o programa 1000 Futuros Cientistas (DQ/UFMG), por meio do projeto 1000FC Pelo Mundo, promove feiras e oficinas itinerantes como recursos pedagógicos para a aprendizagem por investigação e a formação docente. Em 18/10/2025, realizou-se a 1ª Feira de Ciências e Sustentabilidade do Sertão Maranhense (com apoio do CNPq), com foco na iniciação científica contextualizada e na valorização de saberes locais. O evento registrou mais de 764 inscritos (estudantes e professoras(es) da educação básica, graduandas(os), pós-graduandas(os) e pesquisadoras(es) de diferentes áreas), com predominância do sertão maranhense. Foram apresentados 70 trabalhos científicos, todos desenvolvidos e apresentados por estudantes da educação básica (EF, EM e EJA), sob orientação de professores e com a mentoria de estudantes de graduação vinculados ao 1000FC, durante o desenvolvimento do projeto e na preparação para a comunicação científica. As temáticas articularam ciência, território e sustentabilidade, com destaque para conteúdos de química, como a qualidade da água, a reciclagem de materiais e a química verde. A programação incluiu oficinas formativas (robótica educacional, etnociência, práticas agroecológicas, biodiversidade do Cerrado e produção de foguetes), apoiando a transposição didática para o contexto escolar. Como contribuição para o ensino, a feira organizou um percurso investigativo (problema–hipótese–procedimento–evidências–conclusões–comunicação), mobilizando competências de argumentação, resolução de problemas e comunicação científica, além de favorecer a formação continuada de professoras(es) com propostas replicáveis. Dez trabalhos foram premiados e apoiados para a continuidade, reforçando a iniciação científica como prática educativa e indutora da equidade territorial.



Trabalho apresentado por estudantes durante a Feira

Agradecimentos/Acknowledgments

DQ/UFMG, PROEX/UFMG, PRPq/UFMG, INCTs (Midas, Inibidores de Urease, Substâncias Psicoativas), Redes(Escalab Mineral, Mineira de Biofertilizantes, Mineira de Ciência Forense), CNPq, FAPEMIG, MCTI.

Elementos da Representação Social de Professores Universitários sobre Interações Intermoleculares

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Palavras Chave:*Interações intermoleculares, representação social, teoria do núcleo central, estrutura conceitual*

Highlights

In the social representation of university chemistry professors regarding intermolecular interactions, the strength of the types of interactions and the polarity of molecules are predominant.

Resumo/Abstract

A Teoria do Núcleo Central das Representações Sociais (RS) busca descrever como um objeto é percebido e compartilhado por umgrupo social, destacando o núcleo central (NC), formado pelos conceitos e ideias centrais e estáveis que organizam as demais ideias e o sistema periférico (SF), ideias suscetíveis a mudanças. Neste trabalho descrevemos a estrutura da RS de docentes atuantes na área de Química em diferentes IES a respeito do tema Interações Intermoleculares (Int).

114 docentes responderam a um teste de associação livre de palavras onde cada participante lista e ordena as cinco primeiras palavras que lhe vêm à mente diante do termo indutor (Int). Foram calculadas a frequência (F) e ordem média de evocação (OME - a média da posição de cada palavra após sua hierarquização), considerando os 50% termos mais frequentes (20 termos distintos). Conceitos com baixa OME e alta F são considerados os mais salientes (S). Já a conectividade (C) indica como conceitos mais centrais aqueles mais conectados (citados conjuntamente) com outros. Um possível núcleo central é obtido pela intersecção entre S e C. Os demais compõem as periferias.

Resultados: 1) O termo de maior destaque é Ligação de Hidrogênio (F=67, OME=2,55 e C=158), seguido de um grupo formado por Interação de van der Waals (F=31, OME=2,9 e C=29), Polaridade (F=25, OME=2,64 e C=23) e Dipolo (F=21, OME=2,86 e C=24); 2) Forças de Dispersão (F=23, OME=3,70 e C=21) se destaca pela C e F, mas apresenta baixa OME; 3) Polarizabilidade (F=7, OME=2,29 e C=5), uma propriedade importante, foi lembrada por poucos, mas foi considerada importante por estes (baixa OME).

Conclusão: O possível NC dos docentes é composto por: Ligação de Hidrogênio (maior destaque), Interação de van der Waals e Forças de Dispersão – tipos de interações, Dipolo e Polaridade – propriedades moleculares. No SF se destacam conceitos referentes a propriedades das substâncias, polarizabilidade, estrutura molecular, ligação química e outros tipos de interação.



Conectividade - Árvore de máxima similitude

Agradecimentos/Acknowledgments

Aos professores que gentilmente responderam a esta pesquisa.

Ensino de Cinética Química com Arduino e sensor de CO_2: uma proposta contextualizada para o Ensino Médio Integrado ao curso técnico de Automação Industrial

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Palavras Chave:*: Cinética Química,Ensino Médio Técnico,Arduino,Sensor,Tecnologia.*

Highlights

1Chemical Kinetics teaching in integrated technical high school.

2Monitoring the acetic acid–bicarbonate reaction using a CO_2 sensor and Arduino.

3Real-time data collection and graph analysis

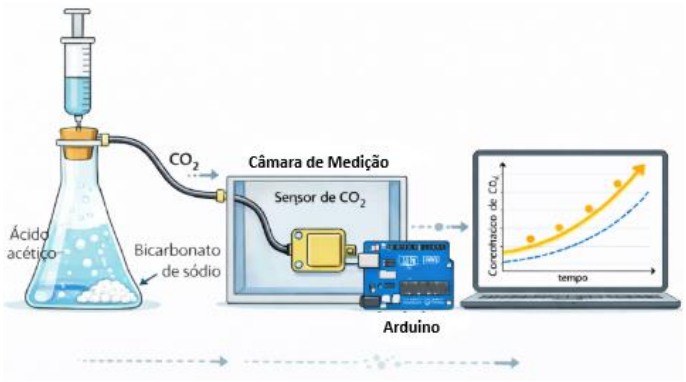
Resumo/Abstract

No contexto do Ensino Médio integrado à Educação Profissional e Tecnológica, os conteúdos de Química frequentemente são abordados de forma pouco articulada à formação técnica dos estudantes, o que pode dificultar a compreensão de suas aplicações em contextos tecnológicos. Nesse cenário, este trabalho investiga como a integração entre conceitos de Cinética Química e ferramentas tecnológicas utilizadas no curso técnico de Automação Industrial pode contribuir para o processo de ensino e aprendizagem dos estudantes.

A pesquisa envolve o desenvolvimento de uma sequência didática fundamentada na Aprendizagem Baseada em Problemas (ABP), estruturada a partir de uma situação-problema inspirada no contexto de uma fábrica automatizada. Para solucioná-la, os estudantes investigam fatores que influenciam a velocidade das reações químicas, com destaque para a concentração dos reagentes.

Como parte do processo investigativo, foi desenvolvido um sistema experimental automatizado utilizando um sensor de gás acoplado a um microcontrolador Arduino para monitorar, em sistema fechado, a reação entre ácido acético e bicarbonato de sódio, responsável pela liberação de dióxido de carbono (CO_2). O sistema permite a coleta de dados em tempo real e a geração de gráficos para análise das curvas cinéticas.

A pesquisa encontra-se na etapa metodológica anterior à aplicação em sala de aula, envolvendo a validação técnica do protótipo e a organização do material instrucional. Testes experimentais preliminares demonstraram que o sensor apresenta sensibilidade adequada para monitorar a variação da concentração de CO_2 em tempo real, permitindo a análise das curvas cinéticas e evidenciando a influência da concentração inicial na velocidade da reação. Esses resultados indicam que o sistema desenvolvido apresenta robustez técnica e potencial para investigar, em etapa posterior, o processo de ensino e aprendizagem de Cinética Química no Ensino Médio Técnico.



Esquema do sistema experimental proposto na sequência didática.

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Environmental education and Chemistry training: The presence of environmental dimensions in chemistry courses based on articles from Latin America

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Palavras Chave:*Environmental Education,chemistry courses,environmental dimension,curriculum*

Highlights

Training chemists means going beyond essentially technical aspects and integrating the environmental dimension into curricula, which is essential for critical, ethical, and sustainable action.

Resumo/Abstract

During chemistry training, there is a predominance of technical teaching, which, in many cases, gives little prominence to socio-environmental discussions, raising questions about the responsibilities of professional chemists and the inclusion of these topics in undergraduate courses. Kistemacher and Costa (2022) highlight the importance of incorporating environmental dimensions into educational processes, including higher education, as a fundamental element in training critical and socially committed professionals. In this context, the study aimed to observe how the environmental dimension has been incorporated into chemistry courses in Latin America, based on a bibliographic review of scientific articles indexed in the SciELO and Web of Science databases. Bibliographic research was adopted because it allows for the collection, analysis, and systematization of previously published scientific works, a fundamental procedure for understanding and deepening knowledge of specific topics (GIL, 2008). Thus, the selection of articles involved screening by titles, keywords, and abstracts, followed by a comprehensive analysis of the texts, resulting in a corpus of 20 articles. The results indicate that publications focus on the discussion of environmentalization of curricula, followed by proposals for sustainable teaching experiments and environmental education workshops in initial teacher training. Although studies reveal growing concern about training chemists who are more attuned to socio-environmental issues, research on the inclusion of these issues in higher education in chemistry in Latin America remains limited, underscoring the need to expand research and training proposals that consistently integrate environmental education into the curriculum.

Agradecimentos/Acknowledgments

LAPEQUIM - Chemistry Education Research Laboratory – UNIFAL-MG. CAPES

Escape Room Científico: uma proposta lúdica e interativa para divulgar a Química e outras Ciências avaliada pelos Resultados Genéricos da Aprendizagem

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Palavras Chave:*Divulgação Científica,Ludicidade,Resultados Genéricos da Aprendizagem,Extensão Universitária*

Highlights

Generic Learning Outcomes reveal conceptual and attitudinal learning in an immersive science escape room. The game promotes engagement with science and exposes alternative conceptions about chemistry.

Resumo/Abstract

O projeto Escape Room Científico (ERC) surgiu como uma ação de divulgação científica (DC), articulada à extensão, voltada ao engajamento do público com as Ciências de forma lúdica, interativa e colaborativa. O presente trabalho busca compreender as experiências vivenciadas pelos participantes à luz dos Resultados Genéricos da Aprendizagem (RGA) e possíveis concepções alternativas associadas aos enigmas químicos. Entre os conteúdos químicos abordados nos desafios do jogo, destacam-se a interação da luz com a matéria e a leitura e interpretação de dados da tabela periódica. A pesquisa adotou uma abordagem qualitativa, baseada na análise das respostas a um questionário aplicado aos participantes após a vivência no jogo. O questionário contém questões dissertativas e outras em escala Likert. Para a questão dissertativa “Conte-nos alguma coisa que você tenha aprendido e/ou desenvolvido durante a sua participação no Escape Room”, os participantes relataram aprendizagens associadas às cinco dimensões dos RGAs — conhecimento e entendimento; habilidades; valores e atitudes; prazer, inspiração e criatividade; e ação, comportamento e progressão (Hooper-Greenhill, 2007) — evidenciadas em falas como “Relembrei conhecimentos sobre a tabela periódica”, “Raciocínio lógico”, “Aprendi que é importante escutar o grupo para ajudar a desvendar as pistas”, “Criatividade”, “A tentar lidar com os problemas sob pressão”. Para a questão “Um material pode ser classificado como translúcido, transparente ou opaco e não depende da interação com a luz”, 54,4% dos participantes concordaram totalmente, enquanto 17,8% discordaram totalmente, indicando concepções ainda pouco consolidadas. Os resultados apontam que o ERC promoveu engajamento e aproximação com a ciência, além de evidenciar a pertinência dos RGAs como ferramenta avaliativa em ações de DC. Ademais, as concepções alternativas observadas nas respostas reforçam a relevância da DC para a reflexão crítica.



Imagens do Escape Room Científico

Agradecimentos/Acknowledgments

Agradecemos à FAPEMIG pelo apoio e financiamento desta pesquisa, aos colaboradores do projeto de extensão vinculado ao Escape Room científico e à equipe do Centro de Ciências da UFJF.

Evaluating One Year of Green Chemistry at The University of Hawaii - Maui College: Institutional Impact and Pedagogical Outcomes

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Palavras Chave:*Green Chemistry, Pedagogical Innovation, Institutional Sustainability, Hawaii, Waste-Mitigation,Green Chemistry, Pedagogical Innovation, Institutional Sustainability, Hawaii, Waste-Mitigation,Green Chemistry,Pedagogical Innovation,Sustainability,Hawaii*

Highlights

Evaluates a year of Hawaii's first Green Chemistry Commitment. Findings include significant reductions in hazardous effluent, enhanced student technical proficiency, and modernized research curricula.

Resumo/Abstract

In April 2025, the University of Hawaii Maui College (UHMC) became the first institution in Hawaii to sign the Beyond Benign Green Chemistry Commitment (GCC). This initiative connects UHMC with a global network of scientists working to make chemistry more sustainable by focusing on waste prevention, the use of safer chemicals, and energy efficiency. This presentation reviews the institutional and educational results observed during our first year of full integration.

Transitioning to a "green chemistry" curriculum required a thoughtful update of traditional laboratory protocols. By following the GCC framework, our STEM department successfully replaced several high-waste experiments with safer, more sustainable alternatives. This shift has not only lowered the environmental impact of our labs but has also helped reduce long-term costs associated with hazardous waste management.

Beyond the environmental benefits, we found that this integration is a powerful tool for student development. By learning modern, sustainable practices, students develop the critical thinking skills and technical expertise needed in today's workforce. We will present a clear analysis of:

Specific changes made to General and Organic Chemistry lab experiments.

Results from student assessments regarding their awareness of environmental safety and chemical life cycles.

How this sustainable model can be adapted by other colleges in geographically isolated regions like Hawaii.

As the first campus in the islands to take this step, UHMC serves as a model for how colleges can modernize science education. Our experience shows that adopting these standards protects our local environment while better preparing students for future careers.

Agradecimentos/Acknowledgments

The authors thank the UHMC STEM Division Chair, Sean Calder and the Beyond Benign community for the resources and support needed to launch the Green Chemistry Commitment in the state of Hawaii.

Evaluating Question-Asking skill in Higher Education through assessment refinement: a case study about chemical bonding learning

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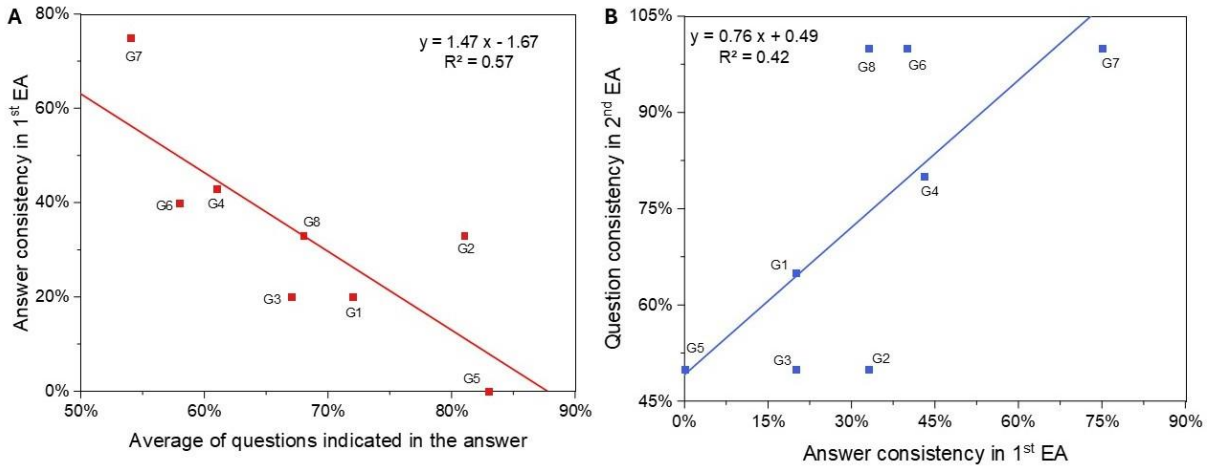
Palavras Chave:*Assessment,Chemistry education,Chemical Bonding,Higher Education,Question-Asking*

Highlights

Through assessment refinement, this case study evidences that the learning of question-asking skills is related to the ability to analyze in detail parts of a problem.

Resumo/Abstract

This research aims to develop question-asking skills, through formative assessments (FA) applied at the discipline “Chemical bonding beyond classical models”, in the Bachelor of Chemistry course in USP Ribeirão Preto. The question-asking skill is a higher order cognitive skill (HOCS) linked to the development of other HOCS such as problem solving and system thinking (related to the ability to solve a problem (system) through analysis of its parts (subsystems)) (Zoller, Levy Nahum*Springer Int. Handb. Educ.*, 2012). Two essay activities (EAs) were applied, in class and in groups, to 34 undergraduates. In the 1st EA, students should answer a complex question guided by 12 (I – XII) provided simpler questions (answering all 12 was not mandatory). In the 2nd EA, students should elaborate their own complex question following the 1st EA’s model, creating at least 5 simpler questions. When revisiting the “question-asking” model in both activities, assessment refinement (an aspect of FA) was implemented (Holme*et al.*,*Chem. Educ. Res. Pract.*, 2010). Analyzing the answers in 1st EA (Figure A), it was diagnosed that groups (G1 – G8) who attempted to answer the greatest number of simpler questions tended to be less consistent (*e.g.*students indicate that they answered questions I to X, but their text does not contain the contents of questions V and X (80% of answer consistency)). In general, groups with higher consistency in 1st EA elaborated better questions in 2nd EA (Figure B). In the 2nd EA “Question consistency” was measured through analysis of coherence between the complex question and the simpler questions (*e. g.*100% of consistency means that all simpler questions elaborated allow to build the answer for the complex question created). Conclusively, the relationships shown in Figures A and B evidence that question-asking learning is more related to the ability to analyze in detail few parts of a problem, rather than trying to analyze the whole problem superficially.



Relationships between diagnoses in 1st EA (A) and 2nd EA (B)

Agradecimentos/Acknowledgments

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Evasão e permanência na Licenciatura em Química (2015–2025): um relato de experiência à luz de Pierre Bourdieu

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Palavras Chave:*Habitus Clivado; Licenciatura em Química; Políticas Institucionais*

Highlights

Account of experience articulated with institutional dropout data: discrepancies between institutional expectations and objective living conditions in a Chemistry Licentiate degree.

Resumo/Abstract

Este trabalho articula um relato de experiência de licenciando em um curso de Licenciatura em Química de uma IES pública com dados de uma pesquisa institucional sobre evasão no curso entre os anos de 2015 e 2025. A análise combina escrita reflexiva e referenciais de Pierre Bourdieu, especialmente os conceitos de*habitus*, capitais, campo e violência simbólica, para compreender a evasão como problema estrutural e não meramente individual. Na Figura 1 observa-se a distribuição da situação acadêmica dos estudantes da Licenciatura em Química no período de 2015 a 2025, evidenciando alta taxa de exclusão/evasão (56%), estudantes ativos no sistema (19,5%), graduados (14%), trancados (7,5%) e formandos no momento da coleta (3,1%). O relato do estudante egresso da escola pública, que também era trabalhador no período de ingresso no curso, explicita como a dupla jornada, a escassez de tempo, as dificuldades de acesso a políticas de assistência estudantil e a opacidade das regras acadêmicas obstacularizam o processo, chamado por Bourdieu (2004) de*habitus clivado*, que pode ser entendido como o rompimento de barreiras de origem social para alcance do sucesso intelectual. A partir da noção de violência simbólica, vivenciada pelo estudante, argumenta-se que a naturalização do fracasso e da evasão no curso de Química contribui para a reprodução das desigualdades educacionais, mesmo em contextos de expansão do acesso ao ensino superior. Identifica-se, contudo, a presença de*illusio*, o investimento no valor simbólico da formação em Química, e de estratégias coletivas de resistência, como redes informais de apoio entre estudantes, grupos de estudos, apoio de alguns docentes e monitorias, citados no relato do estudante. Políticas institucionais devem considerar os desajustes sociais sob pena de a evasão operar como mecanismo silencioso de exclusão de vidas marcadas por descompassos entre expectativas institucionais e condições objetivas de existência.

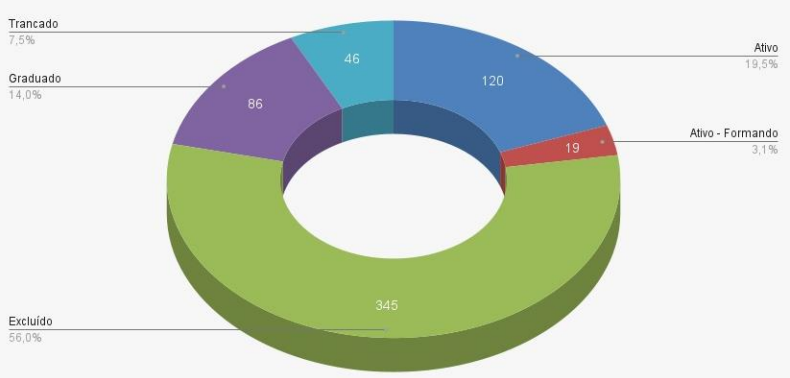


Figura 1 - Situação acadêmica dos estudantes da Licenciatura em Química no período de 2015 a 2025

Agradecimentos/Acknowledgments

À Coordenação de Licenciatura em Químcai da Universidade Federaç de Goiás.

Experiências formativas: visita técnica aos laboratórios do IFPI por alunos de ensino médio no contexto do PIBID

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Palavras Chave:*Visita técnica, PIBID, Aprendizagem significativa*

Highlights

Technical visit to IFPI laboratories. To observe the laboratory routine and the academic reality. Acid-base extraction of lapachol. Meaningful learning outside the classroom

Resumo/Abstract

O PIBID é um espaço formativo ideal para inovações por parte dos bolsistas, pois permite o desenvolvimento de diferentes estratégias de aprendizado, essenciais para o perfil profissional docente. Nesse contexto, foi organizada uma visita técnica para alunos de 3ª série aos laboratórios de química do IFPI – Teresina Central com o objetivo de aproximar os estudantes da rotina de laboratório e da realidade acadêmica, que muitos assumiram não conhecer. Durante a visita, puderam conhecer equipamentos e projetos dos laboratórios de Química Orgânica e de Biomateriais, contudo, a verdadeira experiência formativa ocorreu no laboratório de Química Geral, onde puderam realizar a extração ácido-base do lapachol, composto associado à cor das flores do ipê – árvore símbolo do estado do Piauí. Para a prática, buscou-se atingir os conhecimentos prévios dos alunos, inicialmente sobre o ipê e seu significado para o Piauí e, posteriormente, sobre boas práticas no laboratório de química, como medidas de segurança e nomes de algumas vidrarias – especialmente as que seriam utilizadas. Apesar de dificuldades inicias e certa falta de atitude, os alunos, divididos em grupos, seguiram com a prática e realizaram pesagens em balança analítica, medições de volume com proveta, pipetaram HCl na capela, filtrações e, por fim, preparam solução etanólica de lapachol para ser usada como indicador ácido-base no laboratório. A visita aos laboratórios concretizou um momento de aprendizagem significativa fora da sala de aula, despertando o interesse de alguns alunos pelo ambiente universitário. Também vale pontuar as contribuições para a formação dos licenciandos que conduziram a visita e a prática no laboratório, pois levar alunos da escola-campo para o Instituto favoreceu momentos de exercício da prática docente com novas abordagens. Portanto, a visita técnica contribuiu para a formação científica dos alunos de 3ª série, bem como para a formação inicial dos licenciandos.



Alunos no laboratório de Química Geral realizando a prática de extração do lapachol.

Experimentação para preparação de um produto final no Ensino Técnico Integrado em Química por meio da Produção de Cosméticos com Ativos Naturais

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Palavras Chave:*Ensino,Experimentação,Cosméticos,Ativos naturais*

Highlights

Aprendizagem de Química por meio de projetos experimentais. Projetos com uso de ativos naturais para a produção de cosméticos naturais com nome e identidade visual.

Resumo/Abstract

A experimentação constitui um elemento central no ensino de Química, pois favorece a integração entre teoria e prática e estimula o protagonismo discente. Este trabalho descreve uma experiência didática desenvolvida com alunos dos terceiros anos do curso Técnico em Química do Ifes – Campus Aracruz, com o objetivo de promover a aprendizagem significativa por meio da preparação de cosméticos capilares utilizando ativos naturais. A metodologia envolveu a identificação dos interesses dos estudantes, o planejamento das atividades, o levantamento dos materiais necessários e a execução dos experimentos laboratoriais durante as aulas práticas e, quando necessário, no contraturno. Os alunos participaram de todas as etapas do projeto, desde a pesquisa das formulações, extração de matérias-primas naturais, preparo das formulações, controle das variáveis experimentais e avaliação das características físico-químicas, até a criação do nome e da identidade dos produtos desenvolvidos.Entre os cosméticos produzidos destacam-se a extração do óleo de mamão papaia para formulação de óleo capilar e a preparação de shampoo à base de maracujá e cúrcuma. Essas atividades possibilitaram a aplicação prática de conteúdos como técnicas de extração, preparo de soluções e emulsões, controle de pH, propriedades de tensoativos, estabilidade de formulações e boas práticas de laboratório.Os resultados evidenciaram elevado envolvimento dos estudantes em todas etapas planejamento e execução experimental, maior compreensão da importância da organização prévia das atividades e do cumprimento do cronograma, além do desenvolvimento de autonomia, trabalho em equipe e criatividade. Portanto a produção de cosméticos capilares com ativos naturais constitui uma estratégia eficiente para o ensino, aproxima de aplicações tecnológicas e contribui para a motivação e formação profissional.

Agradecimentos/Acknowledgments

Agradecimentos ao ifes pelo espaço físico e por todos os equipamentos utilizados para o desenvolvimento dos projetos.

From the Classroom to the Laboratory: Introductory Chemistry Workshops with Antibacterial Assays of Essential Oils in High School

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Palavras Chave:*Educação científicaOficinas experimentais; Atividade prática; Microbiologia,Extensão universitária,Educação científica,Oficinas experimentais,Atividade prática,Microbiologia*

Highlights

This work reports outreach workshops with high school students investigating the antibacterial activity of essential oils against*S. aureus* and*P. aeruginosa* strains.

Resumo/Abstract

A limitação de atividades experimentais no ensino de Química em escolas públicas compromete a compreensão de conceitos científicos. Nesse contexto, a extensão universitária constitui estratégia de aproximação entre universidade e educação básica, favorecendo a integração entre teoria e prática no ensino de Ciências. Assim, foi desenvolvido o projeto de extensão “Jovens Cientistas”, vinculado à Universidade Estadual do Sudoeste da Bahia (UESB – Campus Itapetinga), em parceria com dois Colégios Estaduais, com participação de oito estudantes do 3º ano do Ensino Médio. O objetivo foi promover o letramento científico e favorecer a aprendizagem de conceitos de Química por meio de uma sequência didática investigativa em ambiente laboratorial. A proposta foi estruturada em oito oficinas de três horas, abordando segurança e rotinas laboratoriais, estrutura da matéria, estequiometria, funções orgânicas e compostos bioativos. As atividades ocorreram, majoritariamente, nos laboratórios escolares, com apoio do LABMICRO/UESB para práticas microbiológicas. Como atividade integradora, os estudantes avaliaram o potencial antibacteriano de óleos essenciais comerciais pelo método de disco-difusão, estimulando formulação de hipóteses, planejamento experimental, discussão sobre controles e interpretação dos resultados. O acompanhamento da aprendizagem ocorreu por meio de caderno de laboratório, observação das discussões e apresentação científica final. Esses instrumentos evidenciaram apropriação de conceitos químicos e desenvolvimento de habilidades associadas ao pensamento científico, como interpretação de dados, argumentação baseada em evidências e comunicação científica. Os resultados foram socializados em mostra científica aberta à comunidade escolar, fortalecendo a interação entre universidade e escola. A experiência indica que atividades experimentais investigativas contribuem para o ensino de Química ao favorecer participação ativa e contextualização dos conteúdos científicos.

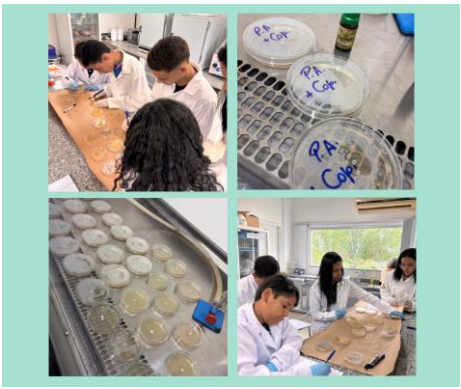


Figura 1. Jovens Cientistas executando atividade antibacteriana com óleos essenciais. Fonte: Autoral

Agradecimentos/Acknowledgments

Agradecemos à UESB–Campus Itapetinga (DCEN/Colegiado de Química e LABMICRO), aos Colégios Estaduais Dutra e Modelo e aos 8 estudantes participantes pela dedicação e parceria.

Gamificação no ensino da estereoquímica: aplicação do jogo “Stereochemistry Race” na graduação em Química

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Palavras Chave:*Ensino de Química,Gamificação,Estereoquímica,Monitoria,Química Orgânica*

Highlights

Aplicação do jogo*Stereochemistry Race*no ensino da estereoquímica de moléculas orgânicas na monitoria de Química Orgânica dos cursos de Química Licenciatura e Bacharelado ICEx-UFF.

Resumo/Abstract

No ensino de química orgânica a temática estereoquímica é um grande obstáculo devido ao seu caráter abstrato, necessidade de domínio dos conteúdos básicos e baixa motivação dos estudantes da graduação em seu estudo. Nesse contexto, o uso de metodologias alternativas, como o ensino por meio da gamificação, promovem o incentivo e o domínio do tema para além do conteúdo introdutório exposto em sala de aula.[1] Diante disso, o presente trabalho apresenta a aplicação do jogo*Stereochemistry Race*(Figura 1), desenvolvido por Júnior e col.,[2,3] no ensino de estereoquímica promovido por meio do projeto de monitoria de Química Orgânica dos cursos de Química Licenciatura e Bacharelado no ICEx-UFF em Volta Redonda. Passível de aplicação para grupos de 2 a 4 jogadores, cada participante deverá percorrer uma trilha composta por 16 casas, sendo distribuídas em 4 núcleos específicos, associados a tarefas determinadas. O objetivo do jogo é alcançar primeiro a área onde se encontra o troféu, tornando-se o vencedor. A dinâmica do jogo baseia-se na resolução correta das questões associadas a diferentes tipos de cartas: vermelhas, contendo afirmações de verdadeiro ou falso; verdes, relacionadas à determinação da configuração absoluta (*R*ou*S*); amarelas, destinadas à classificação das moléculas como quirais ou aquirais; e azuis, voltadas à identificação das relações entre moléculas, como: iguais, isômeros constitucionais, enantiômeros ou diastereoisômeros. Dessa forma, o uso do jogo*Stereochemistry Race*, mostrou-se eficiente tendo em vista que a sua utilização favoreceu o processo de aprendizagem, promoveu o interesse no estudo do conteúdo e em métodos alternativos de ensino, como a gamificação aplicada em outros conceitos da disciplina de química orgânica.

[1] Leite, B. S.;*QNEsc*,**2020**,*42*(2), 147.
[2] Stereochemistry Race – Português em PlayingCards.io, https://playingcards.io/game/stereorace-pt, acessado em janeiro 2026.
[3]Júnior, J. N. S.; et al*Quim. Nova*,**2025**,*48*(5), e-20250132.

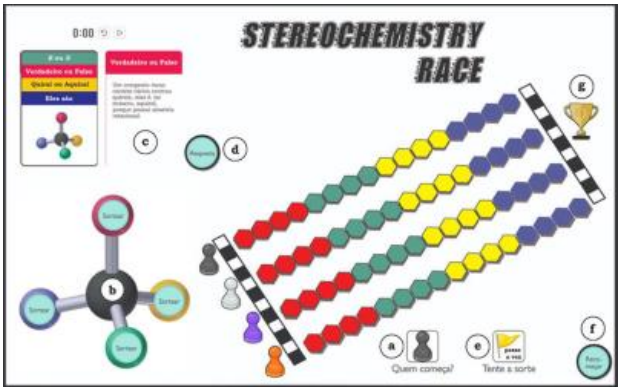


Figura 1. Interface do jogo on-line Stereochemistry Race.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPERJ, UFF.

Gamification of flame testing and audiovisual experimental reporting as a learning strategy in Analytical Chemistry

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Palavras Chave:*Experimentation, investigative learning, gamified classroom.*

Highlights

The flame test was redefined through gamification.

Missions brought students closer to the scientific method and decision-making.

Audiovisual reports increased engagement and conceptual understanding.

Resumo/Abstract

The motivation for applying gamified learning arose as a proposal to make the learning process more active, investigative, and motivating. The flame test experiment, traditionally used in the qualitative identification of cations, was reinterpreted through missions, thematic cards, and a scoring system, bringing students closer to the scientific method and analytical decision-making. This study aimed to promote understanding of the theoretical foundations of flame testing, identify ions present in unknown samples, and stimulate critical thinking and teamwork. The experimental activity was structured in the form of an educational game, in which students, organized into three teams with predefined roles, performed the flame test and completed missions represented by themed cards (Fig 1), such as “Eagle Eye,” “Senior Analyst,” and “Safe Laboratory.” The evaluation considered the observation of the colors emitted, the theoretical interpretation of the results, as well as the organization and conduct of the experiment. The dynamics included scoring, ranking, and formative feedback at the end of the activity. Each team recorded the experimental activity through an audiovisual experimental report, produced in short video format, maintaining the structure of a conventional report (introduction, objectives, theoretical basis, methodology, results, and conclusion). During the “Eagle Eye” mission, students reported interference in the flame test due to impurities and salt residues between samples, highlighting situations in which one ion can mask the identification of another. Only one team made an error in identifying the Ca^{2+} ion. The results indicated high student engagement, better understanding of the relationship between electronic structure and light emission, and improved analytical and collaborative skills. The proposal demonstrates the potential to make experimental Analytical Chemistry classes more meaningful, dynamic, and aligned with active teaching methodologies.

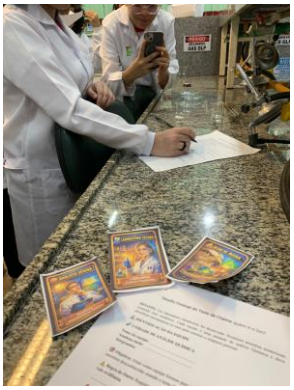


Figure 1 - Execution and recording of the flame test. Detailed mission cards.

Agradecimentos/Acknowledgments

Instituto Federal de Educação Ciência e Tecnologia do Amapá

Gamifying Chemistry: A Practical Guide to Acid-Base Concepts to Engage.

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Palavras Chave:*Active Methodology, Chemistry Teaching, Practical Class and Acid-Base Concept.*

Highlights

Implementation of a teaching sequence based on Active Methodology (Problem-Based Learning and gamification). A practical pH determination lesson with indicators as a central element of engagement.

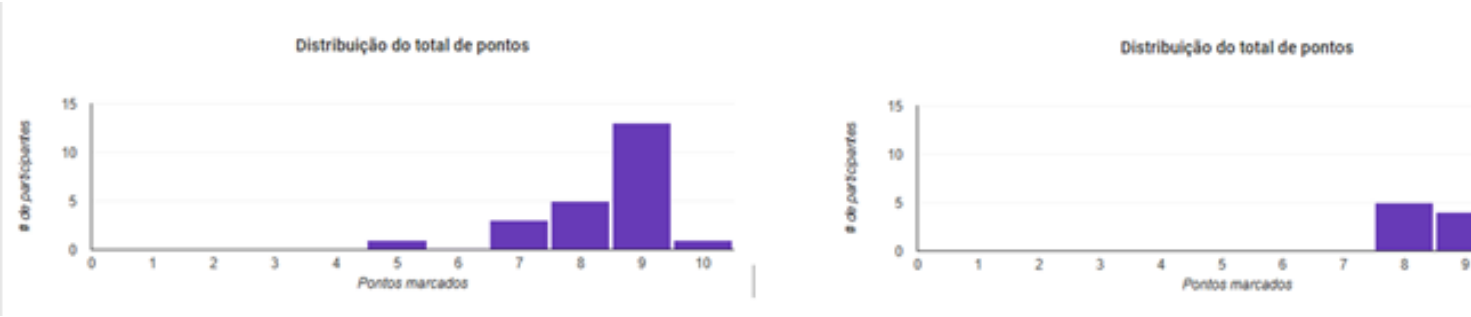
Resumo/Abstract

The teaching of Chemistry, particularly the concepts of acids and bases, often presents significant challenges to students, even being perceived as abstract and decontextualized. This difficulty can lead to demotivation and a superficial learning of the essential fundamentals of chemistry. Given this scenario, the dissertation aimed to analyze the effectiveness of Gamification as an active methodological strategy for teaching and learning the concepts of acids and bases, focusing on the theories of Arrhenius and Bronsted-Lowry.

The research adopted a qualitative and quantitative approach, characterizing itself as action research. The intervention instrument, entitled a practical script, incorporated game elements such as scoring, challenges, and immediate feedback. The application took place with 23 students from the 3th grade of high school in a public school. Data were collected through pre-tests and post-tests to assess cognitive performance, as well as questionnaires for participant perception and observation to analyze engagement and motivation.

The quantitative results indicated a significant improvement in student performance in post-tests, such as an average increase in the success rate, especially in understanding the definitions and neutralization reactions. Qualitative analysis revealed a notable increase in student engagement, active participation, and motivation, with students reporting greater interest in chemistry content. Gamification proved capable of transforming classroom dynamics, making the teaching-learning process interactive and enjoyable.

It is concluded that Gamification establishes itself as a promising and effective pedagogical tool to overcome abstraction barriers in Chemistry Teaching, offering a gamified intervention model that can be replicated and adapted to other curricular contexts, promoting more meaningful and lasting learning.



Before and after test comparison.

Agradecimentos/Acknowledgments

UFPR, DQ/UFPR, PROFQUI, CAPES and SBQ for the opportunity to develop and show this work and the academic community for its continued support of research in Chemistry Education.

ICT in Brazilian Chemistry Education: A Preliminary Review of Proposals in QNEsc

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Palavras Chave:*Keywords: ICT,QNEsc,Chemical Education.*

Highlights

A 30-year review of ICTs in QNEsc shows STSE is the most discussed theme, focusing on High School. Publications peaked between 2020 and 2025, with the Southeast and South regions leading the field.

Resumo/Abstract

The study objective is an analytical overview of proposals about the use of Information and Communication Technologies (ICT) in Brazilian Chemistry Education, based on papers published throughout the 30-year journal history Química Nova na Escola (QNEsc). To this end, a systematic literature review was conducted in May 2025, using the keyword "information and communication technologies" within the QNEsc database. We constructed the corpus in two stages: (1) initial selection of all retrieved files, excluding editorials, indexes, and reviews; and (2) screening of titles, abstracts, and methodologies to identify studies that presented clearly defined ICT proposals or classroom implementations in Chemistry education. Initially, 174 papers were evaluated, resulting in a final corpus of 17 articles. For each paper, we categorized the data according to: (a) core chemistry concepts; (b) target audience; (c) year of publication; and (d) regional origin within Brazil. The articles were systematized into five main themes: Science, Technology, Society, and Environment (STSE) (6), Atomic Theory (4), Chemical Reactions (4), Multi-concept studies (2), and Kinetic Molecular Theory of Gases (1). The prevalence of the STSE theme highlights the significant potential of ICTs to address complex socio-scientific and socio-environmental issues. The majority of proposals were aimed at High School students (9), followed by Higher Education (7) and Technical Education (1). Most publications emerged between 2020 and 2025 (9). Regional output was highest in the Southeast (6) and South (5), followed by the Northeast (3), North (2), and Central-West (1). In summary, the research corpus reveals that ICT proposals in Chemistry Education are with a prominent focus on the STSE approach. Despite this limited breadth, the identified disciplinary and interdisciplinary proposals provide resources for instructional design across various educational levels.

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brazil, Process Number 2024/14351-4 and with support from the National Council for Scientific and Technological Development (CNPq), Brazil, Process Number 153835/2024-9.

Impactos do Programa L'Oréal-UNESCO-ABC Para Mulheres na Ciência na carreira das vencedoras da Química

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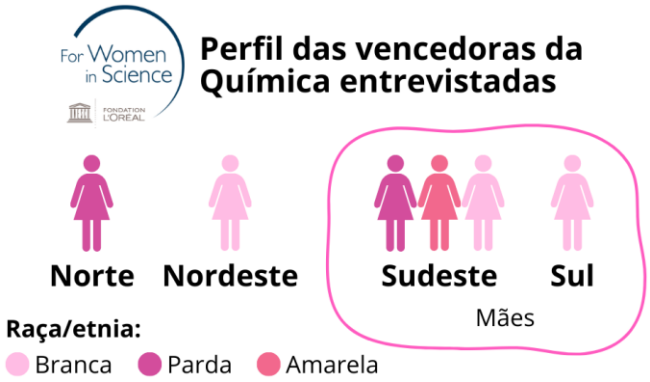
Palavras Chave:*Prêmio L'Oréal, Mulheres na Química, Carreira Científica, Gênero, Trajetória Profissional,Prêmio L'Oréal,Mulheres na Química,Carreira Científica,Gênero,Trajetória Profissional*

Highlights

According to our interviews with six winners of Chemistry of the L'Oréal Awards, receiving the awards consolidated them in the scientific career by providing funding, opportunities and visibility.

Resumo/Abstract

Na Química, as mulheres são minoria nos cargos de professora-pesquisadora e nos patamares mais elevados da carreira, revelando a necessidade de estratégias para reduzir as assimetrias. Assim, o Programa L'Oréal-UNESCO-ABC Para Mulheres na Ciência surgiu no Brasil, em 2006, como uma ação afirmativa cujo intuito é premiar jovens pesquisadoras proeminentes, estando vinculado à iniciativa internacional L'Oréal-UNESCO*For Women in Science*. Nosso objetivo foi analisar os impactos desta honraria no desenvolvimento profissional das vencedoras da Química. Realizamos uma Pesquisa Social Qualitativa, em que constituímos dados nos editais e sites oficiais do programa, bem como nos Currículos*Lattes*das laureadas de 2006 a 2022. Então, entrevistamos seis delas e analisamos os relatos a partir das autoras feministas Heleieth Saffioti, Helena Hirata e Danièle Kergoat. Os resultados apontaram que a maioria das laureadas era proveniente do Sudeste e Sul, todas atuavam em universidades públicas e os projetos premiados se relacionavam a tratamentos de doenças, questões ambientais e desenvolvimento industrial. Com os depoimentos, observamos que a premiação consolidou as entrevistadas na carreira científica. Os principais benefícios do programa foram o recebimento de fomento, que viabilizou melhorias na infraestrutura de seus grupos de pesquisa; as oportunidades surgidas, incluindo possibilidades de circularem em ambientes acadêmicos variados; e a visibilidade, pois, tendo seus nomes divulgados, as laureadas tornaram-se mais conhecidas no meio, aumentando as chances de firmarem parcerias e atraírem estudantes para os grupos de pesquisa. Consideramos esses três aspectos determinantes para que as entrevistadas se estabelecessem cada vez mais no campo e é nítido que o programa transformou a vida delas. Porém, um limite observado diz respeito ao fato de que mesmo tendo se consolidado, as vencedoras ainda lidavam com dificuldades decorrentes do gênero em suas trajetórias profissionais.



Perfil das vencedoras da Química entrevistadas por região geográfica, raça/etnia e maternidade

Agradecimentos/Acknowledgments

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Integração entre Química e Arte em Museus de Ciência: uma análise da oficina GrafittiCCA.

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Palavras Chave:*Interdisciplinaridade, Relação museu-escola, Arte urbana, Reações químicas, Educação não-formal.,Interdisciplinaridade,Relação museu-escola,Arte urbana,Reações químicas,Educação não-formal*

Highlights

Museums and science centers are cultural spaces that enable interdisciplinary dialogue between Chemistry and Art. The GraffitiCCA workshop allowed discussions on Chemistry, urban art, and Sociology.

Resumo/Abstract

A contemporaneidade demanda uma abordagem interdisciplinar que amplie a compreensão da relação entre o ser humano e o conhecimento. A integração entre Arte e Química no contexto educacional favorece a compreensão de conceitos químicos, contribuindo para a desmistificação da Química e despertando interesse e admiração por essa ciência[1]. Nesse cenário, museus e centros de ciência configuram-se como espaços de educação não formal capazes de mediar o diálogo entre Arte e Química, complementando o ensino formal. Este trabalho analisa três edições da oficina “GraffitiCCA”, realizada no Centro de Ciências de Araraquara (CCA), que propõe a integração entre arte, química e educação. As oficinas iniciaram-se com uma introdução ao Graffiti, abordando suas características e relevância social. A 1ª edição contou com a participação de 40 estudantes do 9º ano e resultou na produção de um painel grafitado com o nome do CCA, seguida da aplicação de questionários a alunos e professores. A 2ª edição ocorreu durante a Semana da Química, com estudantes de graduação, utilizando “tintas simpáticas” obtidas por reações entre Fe^{3+} e os ânions $[Fe(CN)_6]^{4-}$, SCN^- e salicilato. Os participantes faziam seus desenhos com as soluções incolores dos ânions e o desenho era revelado com a solução de Fe^{3+}. A 3ª edição repetiu esse formato no evento “Tarde de Férias V”, voltado ao público infantojuvenil. Em todas as edições observou-se o interesse dos participantes em compreender as técnicas da arte urbana e os processos químicos envolvidos, possibilitando discussões sobre pigmentos e reações químicas. Os resultados indicaram maior interesse e melhor compreensão dos conteúdos escolares por parte dos alunos, evidenciando o potencial dos museus de ciência para tornar os conteúdos escolares mais significativos, contextualizado e motivador, fortalecendo a articulação entre teoria e prática no processo de ensino-aprendizagem.
[1] Tenório, O. G.; Marques, J. C. O. N. XIV ENPEC, Caldas Novas – Goiás, 2023



Painel grafitado pelos alunos na primeira edição da oficina "GraffitiCCA"

Agradecimentos/Acknowledgments

Agradecimentos ao Centro de Ciências de Araraquara e IQ-UNESP.

Interdisciplinaridade no Ensino de Química e Bioquímica: O papel da Experimentação investigativa na elaboração de Kit Didático de Biomoléculas

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Palavras Chave:*Análise de dados,Ensino-aprendizagem,Material disruptivo,Observação sistemática,Situação problema*

Highlights

Experimentação investigativa (EI) para o ensino de Química e Bioquímica. Kit didático e práticas experimentais de identificação de Biomoléculas.

Resumo/Abstract

As atividades experimentais, integradas aos referenciais da natureza da Ciência, são centrais no ensino-aprendizagem, articulando a teoria, prática e o desenvolvimento de habilidades científicas essenciais[1]. Todavia, a educação básica brasileira revela limitações quanto ao acesso às práticas experimentais, impactando a formação científica de discentes que ingressam no ensino superior na área das ciências da natureza. Nesse cenário, pesquisas acadêmicas/extensão propõem estratégias didáticas para qualificação da educação básica e para o fortalecimento da interação entre a universidade e sociedade. Dentre as diferentes abordagens experimentais, destaca-se a experimentação investigativa (EI). Fundamentada na proposição de situações-problema que mobilizam os conhecimentos prévios do aluno e incentivam a formulação ativa de hipóteses, observação sistemática, análise crítica de dados e a interpretação dos resultados[2]. Dessa forma, o presente trabalho tem como objetivo central discutir o papel da EI na elaboração de um kit didático voltado à identificação das estruturas e funções das principais biomoléculas especificamente carboidratos, proteínas, lipídios e ácidos nucleicos. O kit foi concebido como uma ferramenta de suporte ao docente do ensino médio, partindo de uma problemática norteadora relacionada à Química e Bioquímica dos alimentos, pautada na reflexão sobre alimentação e nutrição humana. A partir dessa problemática, foram elaboradas atividades de EI específicas para a compreensão estrutural e funcional das biomoléculas citadas. Visando suprir a carência de práticas experimentais acessíveis, o material desenvolvido mostrou-se seguro e adaptável a diferentes infraestruturas escolares. Conclui-se que a EI foi o elemento chave para criação de um material capaz de integrar os conceitos de Química e Bioquímica.

[1]BASSOLI, F.**Ciência & Educação (Bauru)**, v. 20, n. 3, p. 579-593, 2014.

[2]BALDAQUIM, M. J.*et al*.**Actio**: Docência em Ciências, v. 3, n. 1, p. 19-36, 2018.

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Jogos de detetive no ensino de Química: uma revisão da literatura

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Palavras Chave:*Ensino de Química,Gamificação,Jogos de Detetive,Metodologias Ativas*

Highlights

Educational strategies based on detective games and escape rooms have been explored in Chemistry teaching, promoting student engagement, teamwork, critical thinking, and concept review.

Resumo/Abstract

O ensino de Química apresenta desafios relacionados tanto a fatores socioeconômicos e metodológicos quanto à dificuldade dos estudantes em transitar entre os níveis macroscópico, microscópico e simbólico. Nesse contexto, metodologias ativas, como a utilização de jogos pedagógicos, têm sido investigadas como estratégias para favorecer o engajamento discente e o processo de aprendizagem.

Paralelamente, o crescente interesse pela ciência forense, impulsionado por programas de televisão, literatura, filmes e jogos, tem sido explorado no ambiente educacional como elemento motivador. Assim, este trabalho apresenta uma revisão bibliográfica de artigos publicados em periódicos científicos, com foco em jogos de detetive e atividades do tipo Escape Room aplicadas ao ensino de Química, tanto no Ensino Médio quanto no Ensino Superior.

A busca foi realizada utilizando palavras-chave como*game detective, forensic science, whodunit, ChemEscape, ChesRms e investigative game*, considerando publicações disponíveis no Portal de Periódicos CAPES e no*Journal of Chemical Education.*Inicialmente foram identificados diversos trabalhos nas bases consultadas, dos quais 13 estudos atenderam aos critérios de seleção e foram incluídos na análise final. A seleção dos estudos baseou-se na leitura de títulos e resumos, priorizando propostas educacionais que envolvessem a resolução de mistérios ou crimes por meio de desafios relacionados a conceitos químicos. Foram considerados estudos voltados para diferentes níveis de ensino (Ensino Fundamental, Médio e Superior), bem como propostas desenvolvidas em formatos digitais, híbridos ou presenciais.

Os trabalhos analisados indicam que atividades como jogos educativos, especialmente aquelas baseadas em Escape Rooms, Battle Boxes e jogos de interpretação de papéis, favorecem o desenvolvimento do trabalho em grupo, o aprimoramento do senso crítico, a revisão de conteúdos e o aumento do interesse dos estudantes pela Química e pela Ciência.

Agradecimentos/Acknowledgments

As autoras agradecem à UDESC, à FAPESC e à CAPES pelo apoio institucional e financeiro ao desenvolvimento deste trabalho

"Tô Dentro, Tô Fora: Desafiando a Química": jogo didático de cartas para promover aprendizagem colaborativa e argumentação científica no Ensino Médio.

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Palavras Chave:*Ensino de Química; Jogos didáticos; Argumentação científica; Protagonismo discente; Aprendizagem colaborativa*

Highlights

A card-based true/false game enhances conceptual learning, scientific argumentation and student engagement in high school Chemistry through active collaboration.

Resumo/Abstract

Esta pesquisa teve como objetivo desenvolver, aplicar e analisar um jogo didático de cartas com afirmativas denominado*"Tô Dentro, Tô Fora: Desafiando a Química"*, para o ensino de Química no Ensino Médio, investigando seu potencial para mobilizar conceitos, favorecer a argumentação científica e promover a participação e a interação colaborativa entre os estudantes[1]. O jogo é composto por 263 cartas, cada uma contendo uma afirmativa relacionada a conteúdos de Química do Ensino Médio, organizadas por eixos temáticos (Tabela Periódica, Química Orgânica, Bioquímica, Energia e Sustentabilidade e Curiosidades) e níveis de dificuldade. O jogo consiste na análise das afirmativas por grupos de estudantes, que respondem por meio das expressões "Tô dentro!" ou "Tô fora!", indicando, respectivamente, se consideram a proposição verdadeira ou falsa. A metodologia compreendeu o desenvolvimento do material, a aplicação do jogo em turmas de 2º e 3º anos de escolas do Estado do Rio de Janeiro e a análise das interações e decisões dos estudantes. Para o registro sistemático das respostas, foram utilizadas fichas de pontuação e um diário de campo, cujos dados subsidiaram análises quantitativa e qualitativa.

Os resultados indicaram que o uso intencional do jogo potencializou a aprendizagem conceitual, ao estimular a análise crítica, a explicitação de justificativas e a validação do conhecimento científico. Observou-se maior engajamento e capacidade de relacionar conceitos químicos a diferentes contextos, além do fortalecimento da cooperação, comunicação e protagonismo discente. A estrutura do recurso, de baixo custo e fácil aplicação, mostrou-se adequada a diferentes realidades escolares e eficaz como instrumento diagnóstico e de avaliação formativa. Conclui-se que o jogo constitui um produto educacional consistente e replicável, alinhado às diretrizes da BNCC.

1.Bacich, L.; Moran, J.;*Metodologias ativas para uma educação inovadora:uma abordagem teórico-prática*.2018.Porto Alegre: Penso.



Organização pedagógica de uma carta do jogo "Tô Dentro, Tô Fora: Desafiando a Química"

Agradecimentos/Acknowledgments

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Ludicidade e Ensino de Química Orgânica: Desenvolvimento de um RPG de mesa como Recurso Didático

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Palavras Chave:*Química orgânica,Ludicidade,Role Playing Game,Química Orgânica*

Highlights

Playfulness and Organic Chemistry Education: A Tabletop RPG as a Teaching Resource. This work presents a tabletop RPG linking medicinal plants and organic chemistry through ludic learning.

Resumo/Abstract

A elaboração de materiais lúdicos[1] no ensino de Química tem se mostrado eficaz ao aproximar conceitos abstratos da experiência concreta dos estudantes. No ensino de Química Orgânica[2], essa abordagem é ainda mais relevante diante das dificuldades relacionadas à visualização estrutural, compreensão de propriedades e aplicação prática dos conteúdos. Neste trabalho, descrevemos a criação de um*Role Playing Game*(RPG)[3] de mesa como recurso didático, integrando narrativa, experimentação e elementos da biodiversidade brasileira. A metodologia baseou-se na análise documental qualitativa do acervo de plantas medicinais da exposição*Pharmacia*do Museu da História da Medicina do Paraná, seguida da classificação dos fitoterápicos e da elaboração dos componentes do jogo. As cartas compõem o núcleo lúdico-pedagógico e atuam como mediadoras entre a narrativa e os conceitos químicos. Foram produzidos cinco tipos principais: (1) Cartas de Plantas Medicinais, com dados botânicos e químicos; (2) Cartas de Composição Química, contendo estruturas, funções e propriedades; (3) Cartas de Procedimentos Experimentais, relacionadas a técnicas de extração na Química Orgânica; (4) Cartas de Personagens, que permitem ao estudante escolher papéis dentro da narrativa (Aprendiz, Mestre Alquimista, Botânica, Historiadora, Exploradora ou Viajante do Tempo), cada qual com habilidades específicas; e (5) Cartas de Doenças, que introduzem desafios adicionais vinculados à necessidade de identificar princípios ativos. A organização das cartas materializa as relações planta, composto, técnica, interpretação química e ação narrativa, favorecendo conexões significativas e a aplicação ativa do conhecimento científico. Os resultados indicam que o RPG de mesa apresenta grande potencial como ferramenta lúdica para o ensino de Química Orgânica, ampliando o engajamento dos estudantes, promovendo aprendizagem significativa e integrando diferentes dimensões da ciência de forma acessível e motivadora.

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Maker-Based Digital Calorimeter: Developing a Low-Cost Educational Tool for Chemistry Teaching in Remote Areas

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Palavras Chave:*Calorimetry,Chemistry education,Maker culture,3D printing,Open technologies*

Highlights

A digital calorimeter built with accessible technologies and maker culture integrates chemistry, electronics, and coding in a technical course in a remote region of Amazonas, Brazil

Resumo/Abstract

Teaching Chemistry in Brazilian public schools faces several challenges, including scarcity of educational resources, limited laboratory infrastructure, and infrequent experimental activities. In remote areas with Indigenous communities, such as the interior of Amazonas State, these issues are even more pressing, highlighting the urgent need for creative and affordable solutions. In this context, maker culture and open-source communities have emerged as viable alternatives for developing customizable educational tools that integrate multiple knowledge areas and address diverse learning environments. This study presents the development of a digital calorimeter for educational purposes, created using accessible technologies such as Arduino, a digital temperature sensor, and 3D printing. The prototype was designed within an interdisciplinary project developed by students from a technical program in Information Technology in São Gabriel da Cachoeira, Amazonas, Brazil, as an alternative to the traditional supervised internship. The initiative combined electronics, coding, and 3D modeling with core concepts of physical chemistry. Temperature measurements were taken using an Arduino Uno microcontroller and a DS18B20 digital sensor, with real-time data visualization via custom software currently under development. Experimental validation, based on monitoring temperature variations in documented chemical reactions, is ongoing as the final of this project. This proposal aims to contribute to Chemistry education with a hands-on, low-cost, and replicable approach aligned with active learning methodologies. Moreover, it promotes student engagement and interdisciplinarity in technical education, particularly in underserved regions, through the pedagogical use of open technologies.

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Marie Curie e a Federação Brasileira pelo Progresso Feminino em São Paulo (1926): potencialidades para o Ensino de Química e Popularização da Ciência

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Palavras Chave:*Marie Curie, Federação Brasileira pelo Progresso Feminino, Popularização da Ciência, Ensino de Química*

Highlights

Historical records of Marie Curie's 1926 visit to São Paulo are analyzed through women's scientific and political networks, highlighting potential for teaching Chemistry and popularizing science.

Resumo/Abstract

Em 1926, Marie Curie visitou o Brasil a convite do Instituto Franco-Brasileiro de Alta Cultura. Entre os dias 13 e 15 de agosto, esteve em São Paulo acompanhada por uma comitiva de mulheres da Federação Brasileira pelo Progresso Feminino (FBPF). A passagem da cientista pelo estado constitui um episódio relevante para a Popularização da Ciência e para o Ensino de Química, sobretudo quando analisada a partir da atuação feminina em momentos envolvendo instituições e conhecimentos químicos. A pesquisa fundamenta-se em abordagem qualitativa de caráter histórico, com base em fontes documentais primárias, especialmente notícias veiculadas em periódicos brasileiros de 1926, integrando um projeto mais amplo sobre a visita de Marie ao Brasil. Do total de 44 notícias localizadas sobre a visita a São Paulo, 20 mencionam diretamente a comitiva feminina, integrada por Bertha Lutz, Carlota Pereira de Queiroz, Maria Vicentina Pereira de Queiroz e Maria Amália Pinto Bastos, evidenciando sua visibilidade na imprensa. Esses documentos registram a presença da comitiva em visitas à autoridades políticas, instituições científicas (como Instituto Butantan, Faculdade de Medicina e Estação Biológica do Alto da Serra), e na viagem à Águas de Lindóia. No ensino de Química, tais documentos apresentam elevado potencial pedagógico, pois permitem articular conceitos como radioatividade, aplicações médicas e interação ciência-sociedade a contextos históricos concretos. Ao evidenciar a atuação de mulheres em redes científicas e políticas, favorecem uma abordagem que integra noções de gênero e traz à tona a presença feminina na história da ciência. Assim, o uso dessas fontes contribui para uma Química histórica e socialmente contextualizada, voltada à Popularização da Ciência, ampliando o diálogo entre escola, sociedade e memória científica nacional, especialmente no contexto do centenário da visita de Marie Curie ao Brasil, em 2026.

Agradecimentos/Acknowledgments

Ao Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq - Processos: 409697/2023-0; 315155/2023-0; 440721/2024-5.

Marie Curie no Brasil: homenagens toponímicas no Estado de São Paulo

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Palavras Chave:*Marie Curie, Homenagens toponímicas, Lugares de memória, Mulheres na Ciência*

Highlights

Mapping of Marie Curie's toponymic tributes in São Paulo, Brazil. Street names analyzed as "Sites of memory" for scientific identity.

Resumo/Abstract

Este trabalho identifica as homenagens à Marie Curie no território brasileiro, com recorte analítico para o estado de São Paulo, investigando como a figura da cientista se inscreveu na geografia das cidades. A materialização da memória social no espaço urbano foi compreendida a partir do conceito de "Lugar de Memória", fundamentado em Pierre Nora, definindo a homenagem como a criação de pedestais simbólicos que retiram a personalidade do fluxo temporal para servir de identidade coletiva. A pesquisa baseou-se em levantamento documental e buscas em plataformas de geolocalização e de logradouros, como Google Maps, Open Street Map, Correios e IBGE, utilizando variações nominais da cientista como descritores. Analisaram-se os dados obtidos sob a ótica das homenagens toponímicas, categoria que designa a nomeação de lugares públicos e que, para sua efetivação, respeitou a Lei Federal nº 6.454/1977. Observou-se que esta legislação proíbe atribuir nomes de pessoas vivas a bens públicos, exigindo que a homenageada fosse falecida e que houvesse a tramitação de um projeto de lei ou decreto, mediante a apresentação de uma justificativa biográfica que comprovasse a relevância social ou científica perante o poder legislativo local. Identificaram-se logradouros em 11 municípios: Águas de Lindóia, Araras, Campinas, Guarulhos, Limeira, Lorena, São Bernardo do Campo, São José do Rio Preto, São Paulo, Ubatuba e Amparo. Verificou-se, nestas localidades, a predominância da variação "Rua Madame Curie" em detrimento de "Marie", refletindo o tratamento social dispensado a ela. A nominação está presente em alamedas e chácaras, denotando ampla capilaridade urbana. Concluiu-se que estas homenagens transcenderam a função de endereçamento, atuando como dispositivos de legitimação que, validados pelo poder público, perpetuaram o reconhecimento da cientista e da ciência química no cotidiano das cidades. Um mapa interativo será elaborado para fins de turismo científico e popularização da ciência.

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Material de apoio pedagógico elaborado para alunos e professores em um kit didático de estrutura e funções de biomoléculas.

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Palavras Chave:*material de orientação,ensino-aprendizagem,kit de experimentos,roteiros experimentais.*

Highlights

Material de apoio pedagógico para um kit didático sobre biomoléculas; materiais de apoio para o processo de ensino-aprendizagem; manuais objetivos em um kit experimental para alunos e professores.

Resumo/Abstract

A experimentação é uma ferramenta didática1 utilizada em sala de aula para auxiliar no processo de ensino-aprendizagem, podendo vir acompanhada de diferentes abordagens de ensino. Neste projeto, utilizou-se uma abordagem investigativa com o intuito de apresentar situações problemas para que os alunos tenham papéis ativos na construção do conhecimento2. Pensando nisso, o EBIOMIC desenvolveu um kit de experimentos educativos, de caráter investigativo, sobre estrutura e função de biomoléculas para uso em aulas de química e bioquímica no Ensino Médio (EM). Neste contexto, o trabalho integra um projeto mais amplo, voltado à elaboração de materiais de apoio ao processo de ensino-aprendizagem. Para isso, foram produzidos quatro materiais de apoio destinados aos docentes, cada um relacionado a uma classe de biomoléculas (proteínas, ácidos nucléicos, lipídeos e carboidratos). Os materiais apresentam conceitos teóricos e experimentos que podem ser conduzidos por meio de três trilhas de aprendizagem: a primeira, de caráter demonstrativo, a segunda, realizada pelos estudantes com o auxílio de roteiros, e a terceira, com enfoque investigativo, em que os alunos serão desafiados a solucionar situações problemas relacionadas à temática dos alimentos. Os kits foram pensados com o intuito de aumento gradativo de dificuldade, possibilitando que os professores escolham qual trilha seguir de acordo com a realidade escolar. Todo o material foi aprovado por docentes da equipe e o projeto passará pela etapa de validação com professores e alunos do EM. Ao contar com materiais 3D e audiovisuais, o kit reúne recursos pedagógicos versáteis. Com isso, suas aplicações se adaptam a diferentes realidades, o que o distingue dos kits tradicionais. Ademais, alinhado à ODS 12, inclui gerenciamento de resíduos e fichas de segurança.
1LEITE, B. S. Educación Química, v. 29, n. 3, p. 61-78, 2018.
2SASSERON, L. H. Ensaio Pesquisa em Educação em Ciências, v. 17, n. spe, p. 49-67, 2015.

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Mini-project for teaching adsorption using biomass-modified silica

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Palavras Chave:*Teaching mini-project,modified silica sol-gel,biomass,adsorption,crystal violet*

Highlights

Immersion in research as a motivational tool for Agro-industrial Engineering students.

Silica sol-gel using biomass as a porogenic agent.

Removal of crystal violet dye from 87.0-97.9%.

Resumo/Abstract

Adsorption is of significant importance in the chemical industry, especially in pollutant removal. Therefore, it is necessary to include it in the training of new professionals, employing pedagogical approaches that have already proven their efficiency. Course-Based Undergraduate Research Experiences (CUREs) are important tools for popularizing academic research within undergraduate courses, providing students with a "taste" of the daily life of a researcher. Therefore, this abstract describes a 4-week mini-project for teaching adsorption focused on silica production. Each student in the Physical Chemistry II course (semester 2025/2, Agro-industrial Engineering - FURG) prepared a different biomass (week #1); produced modified silica using their biomass as a template (week #2); and tested the produced adsorbent in the removal of crystal violet dye from water (week #3). Finally, he presented his results to his colleagues (week #4). The biomasses used were peanut, passion fruit, acacia, cocoa, walnut, cassava, and garlic husks, as well as sugarcane bagasse, butia kernel, and pine needles. Adsorption tests were conducted using the batch technique with readings on a UV-Vis spectrophotometer. The results obtained in dye removal ranged from 87.0% to 97.9%, with the best performance obtained by silica modified from garlic peel. Figure 1 shows some steps of the developed teaching sequence. The proposal to address the topic of adsorption through unprecedented scientific investigation, where students had the freedom to choose their object of study (biomass), had never been tested in this discipline. In summary, the immersion in research provided by the CUREs methodology allowed a re-signification of the theoretical concepts worked on in the Physical Chemistry II course, making them useful tools in problem-solving. Thus, the execution of the didactic proposal contributes to student learning with a reduction in the number of failures: from 55% (2023 and 2024) to 10% (2025).

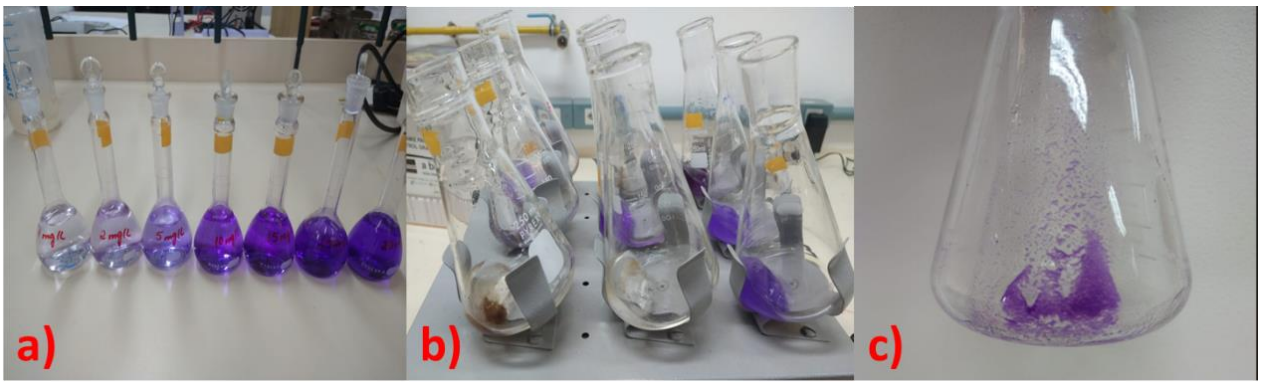


Figure 1. Dye calibration curve (a), adsorption test (b), and the adsorbent with dye (c).

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Narrativas transmídia: contribuições para o desenvolvimento de habilidades de comunicação científica de graduandos em Química

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Palavras Chave:*Transmídia, ensino superior, mídias digitais*

Highlights

The incorporation of digital technologies into Chemistry Education enables a reconfiguration of teaching practices.

Teaching undergraduates to communicate science.

Resumo/Abstract

A crescente inserção de tecnologias digitais na sociedade torna essencial a adoção de estratégias de ensino e aprendizagem associadas a elas. Nessa perspectiva, é promissora a incorporação na Educação em Química de narrativas jornalísticas transmídia (NJT), nas quais os elementos de uma notícia são dispersos de maneira sistemática por múltiplas plataformas de mídia, combinando diferentes meios, linguagens e formatos, para criar uma experiência informativa unificada, coordenada e interativa (RENÓ; FLORES, 2018)[1]. Este trabalho tem como objetivo relatar e analisar a aplicação de atividades didáticas voltadas à produção de NJT por parte dos graduandos em Química, tendo em vista o desenvolvimento de habilidades de comunicação sobre pesquisas científicas para público não especializado. A percepção dos estudantes acerca das atividades desenvolvidas foi também investigada. As atividades foram aplicadas em componente curricular de comunicação científica, em duas turmas, com a participação de 63 estudantes. Foram produzidas 14 NJT, no total, a partir de artigos originais de pesquisa publicados na revista Química Nova. As NJT abordaram temas sobre controle de qualidade de vacinas, ecotoxicidade de cremes dentais, caracterização físico-química de méis e polens e monitoramento da qualidade da água. Todas as NJT apresentaram um meio nativo e foram expandidas por diferentes plataformas midiáticas. Conclui-se que a utilização de NJT se configura como uma estratégia que tem a potencialidade de estimular habilidades de comunicação, criatividade e trabalho em grupo, que são fundamentais para a formação profissional do químico.

1. RENÓ, D.; FLORES, J. Periodismo Transmedia. Ria Editorial, 2018.

Agradecimentos/Acknowledgments

Ao IFBA pela licença capacitação concedida à autora apresentadora deste trabalho e ao (CNPq, Processo 300448/2025-2).

ÓLEOS ESSENCIAIS NO ENSINO DE FUNÇÕES ORGÂNICAS: PROPOSTA DIDÁTICA CONTEXTUALIZADA EM ABORDAGEM CTSA.

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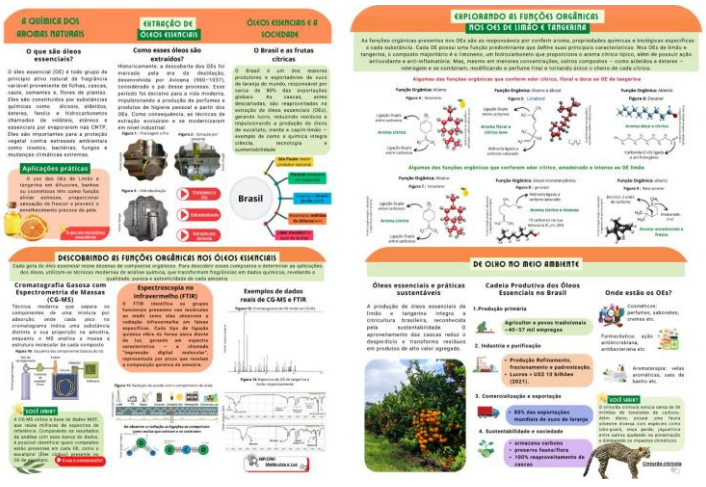
Palavras Chave:*Óleos essenciais,funções orgânicas,abordagem CTSA,ensino de química,contextualização do ensino.,ensino em química,contextualização do ensino*

Highlights

A contextualized educational guide based on essential oils was developed to teach organic functions, integrating scientific data and a CTSA approach to promote meaningful and critical learning.

Resumo/Abstract

A Química, enquanto disciplina da educação básica, assume papel fundamental na formação dos estudantes ao favorecer a interpretação de fenômenos naturais relacionados às transformações da matéria e às suas aplicações cotidianas. Desse modo, o trabalho pedagógico deve pautar-se em situações reais que atribuam sentido e aplicabilidade ao saber escolar, a partir de uma postura construtivista de conceitos. Contudo, o ensino de funções orgânicas ainda é conduzido por abordagens meramente ilustrativas e descontextualizadas. Nesse contexto, questiona-se: como promover um ensino de funções orgânicas significativo e contextualizado? Assim, este trabalho teve como objetivo a elaboração de um produto educacional a partir de dados experimentais obtidos por meio das técnicas de CG-MS e FTIR de óleos essenciais (OEs) de limão e tangerina, para o ensino de funções orgânicas,utilizando a abordagem CTSA. A pesquisa caracterizou-se como mista pela combinação de dados experimentais e pesquisa de campo. A metodologia consistiu na extração e caracterização dos OEs, desenvolvimento de material digital interativo e aplicação em uma turma do 3° ano do ensino médio do IFAL, além da coleta de dados por meio de questionário. Os resultados indicaram que 92,5% dos estudantes reconheceram a química como agente social, tecnológico e ambiental pela aproximação do assunto ao cotidiano. Outrossim, o objeto de estudo aumentou o interesse pelo conteúdo, como exemplificado na fala:“A parte mais interessante é a ideia de que os aromas dos óleos essenciais surgem porque cada molécula tem um tipo de grupo funcional”. Conclui-se que o material didático criado a partir de dados experimentais reais associados à abordagem CTSA promoveu um ensino de funções orgânicas contextualizado, além de una aprendizagem crítica, significativa e próxima da realidade cotidiana dos estudantes.
BRASIL.**BNCC**. MEC, 2018. WHARTA et al.**Cotidiano e contextualização no ensino dequímica**. Química Nova, 2013.



Produto Educacional contextualizado para o ensino de funções orgânicas

Obstáculos no ensino de Química à luz do Triângulo de Johnstone: um estudo de caso com professores e aproximações à noção de conceitos portais

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Palavras Chave:*Conceitos portais, Ensino de Química, Obstáculos de aprendizagem, Mapas conceituais, Triângulo de Johnstone.,Conceitos portais,Ensino de Química,Obstáculos de aprendizagem,Mapas conceituais,Triângulo de Johnstone.*

Highlights

Using concept maps in teacher interviews revealed three core obstacles to learning Chemistry. These obstacles align with Johnstone's Triangle and threshold concepts.

Resumo/Abstract

Este estudo de caso investigou os principais obstáculos no ensino de Química a partir da percepção de nove professores atuantes no ensino médio e superior, com o objetivo de qualificar tais obstáculos à luz de referenciais consolidados e emergentes da área. Foram realizadas entrevistas semiestruturadas online, mediadas por mapas conceituais elaborados e validados pelos próprios participantes, que funcionaram como instrumentos de explicitação e reflexão sobre a prática docente. A análise qualitativa seguiu procedimentos típicos de estudos de caso, combinando análises individuais e comparativas dos mapas conceituais, permitindo identificar recorrências, padrões e convergências entre as representações construídas. A partir dessa análise três dimensões inter-relacionadas emergiram como obstáculos estruturantes à aprendizagem em Química e também se mostraram análogas aos vértices do Triângulo da Química de Johnstone: (1) a dimensão conceitual, associada às dificuldades na compreensão de entidades microscópicas, como átomos e moléculas; (2) a dimensão representacional, relacionada às barreiras impostas pela linguagem simbólica da Química, incluindo fórmulas e equações; e (3) a dimensão operacional, vinculada à dependência do raciocínio lógico-matemático, como proporções e manipulações algébricas. A recorrência e o caráter estruturante dessas dimensões permitem qualificá-las como obstáculos que se aproximam da noção de conceitos portais, organizando e condicionando o avanço conceitual. O estudo reposiciona, assim, o Triângulo de Johnstone como uma lente analítica que dialoga com debates contemporâneos, oferecendo implicações relevantes para o planejamento e a prática docente.

Johnstone, A. H. (2000a).**Chemical Education Research: Where from Here?**University Chemistry Education, 4(1), 34-38.

Correia, P. R. M. et al. (2023).**Threshold Concepts as a Missing Piece Needed to Frame Teaching in Analytical Chemistry.**Journal of Chemical Education, 100(4), 1419–1425.

Agradecimentos/Acknowledgments

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O Ensino de Química na Perspectiva Ciência-Tecnologia-Sociedade

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Palavras Chave:*Educação CTS,Ensino de química,Natureza da ciência*

Highlights

Compreendendo ciência e tecnologia por meio do ensino de Química; Articulando o conhecimento científico a contextos sociais e tecnológicos; Ensinar Química para além das fórmulas.

Resumo/Abstract

A perspectiva Ciência, Tecnologia e Sociedade (CTS) tem se consolidado como uma abordagem relevante no ensino de Química, sendo pertinente compreender como estratégias didático-pedagógicas fundamentadas nessa perspectiva vêm sendo discutidas na literatura da área. Assim, o presente trabalho tem como objetivo mapear e analisar estratégias didático-pedagógicas fundamentadas na perspectiva de educação CTS evidenciadas na literatura de ensino de Química, com vistas à superação de concepções distorcidas sobre ciência e tecnologia. Trata-se de uma pesquisa qualitativa, de caráter exploratório e bibliográfico, desenvolvida por meio de uma revisão sistemática da literatura, orientada pela metodologia PRISMA. O corpus foi constituído por produções acadêmicas publicadas entre 2010 e 2026, localizadas no Portal de Periódicos CAPES a partir dos descritores “ensino de química” e “CTS”. Inicialmente, foram identificados 82 artigos, posteriormente selecionados conforme critérios de inclusão e exclusão previamente definidos. Os dados foram organizados em planilhas e analisados de forma qualitativa. Os resultados indicam que, entre 2010 e 2016, a produção acadêmica sobre CTS no ensino de Química foi baixa e irregular. A partir de 2017, observa-se crescimento progressivo, com pico entre 2019 e 2022, especialmente em 2021, sugerindo ampliação do interesse acadêmico pela abordagem CTS, possivelmente associada a debates curriculares e reformas educacionais. Embora haja redução nas publicações a partir de 2023, a tendência geral aponta para a consolidação do campo. Sendo assim, conclui-se que a educação CTS no ensino de Química tem se fortalecido ao longo do tempo, revelando potencial para promover práticas pedagógicas mais contextualizadas e críticas, contribuindo para uma compreensão mais integrada da ciência, da tecnologia e de suas implicações sociais.

SANTOS, W. L .P ; MORTIMER, E.**Ensaio: Pesquisa em Educação em Ciências**, v.2, n. 2, p. 1-23, 2002.

O JOGO DE RPG COMO ESTRATÉGIA PARA O ENSINO DE QUÍMICA ORGÂNICA

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Palavras Chave:*Educação Química, Gamificação, RPG educacional, Química Orgânica, Ensino Médio,Educação química,Gamificação,RPG educacional,Química orgânica,Ensino médio*

Highlights

Gamification, especially through RPGs, is explored as a strategy to promote student engagement in Organic Chemistry.

A simplified RPG system adapted for 50-minute classes was developed.

Resumo/Abstract

O ensino de Química apresenta desafios relacionados ao interesse e à compreensão dos conteúdos por parte dos estudantes, o que tem motivado a busca por novas estratégias pedagógicas. Nesse contexto, as metodologias ativas vêm sendo investigadas como alternativas para qualificar o processo de ensino e aprendizagem, entre elas a gamificação. Um dos recursos associados a essa abordagem é o RPG (Role Playing Game), contudo, muitos sistemas existentes são complexos e de difícil adaptação à realidade da sala de aula, especialmente em aulas com duração de 50 minutos.

Diante disso, o objetivo deste trabalho foi desenvolver um sistema de RPG simplificado capaz de abordar conteúdos de química orgânica de forma atrativa e pedagogicamente viável. A proposta foi elaborada no âmbito de um Trabalho de Conclusão de Curso, consistindo no desenvolvimento de uma intervenção pedagógica para o Ensino Médio.

O jogo foi planejado para se adaptar às necessidades do professor e possibilitar a abordagem de diferentes conteúdos, sendo possível utilizá-lo para acompanhar a evolução do discente no contexto do jogo, por meio de pontos de ciência (XP), permitindo ajustar a progressão das classes dos personagens, conforme os diferentes anos do Ensino Médio.

A dinâmica do RPG apresenta uma narrativa base no estilo*escape room*, passível de adaptações, na qual os estudantes avançam por salas ao resolver questões e desafios conceituais. O material inclui fichas para criação de personagens, um livro de regras e monstros didáticos fundamentados em conceitos de Química Orgânica, como nucleófilos e eletrófilos (Figura 1), além de três classes temáticas: alquimista, pesquisador e estagiário. A proposta configura-se como uma estratégia pedagógica atrativa para os discentes, que pode estimular maior disposição para a participação nas atividades e a aproximação com os conteúdos de Química, além de dialogar com competências previstas na BNCC, como criatividade, proatividade e tomada de decisão.

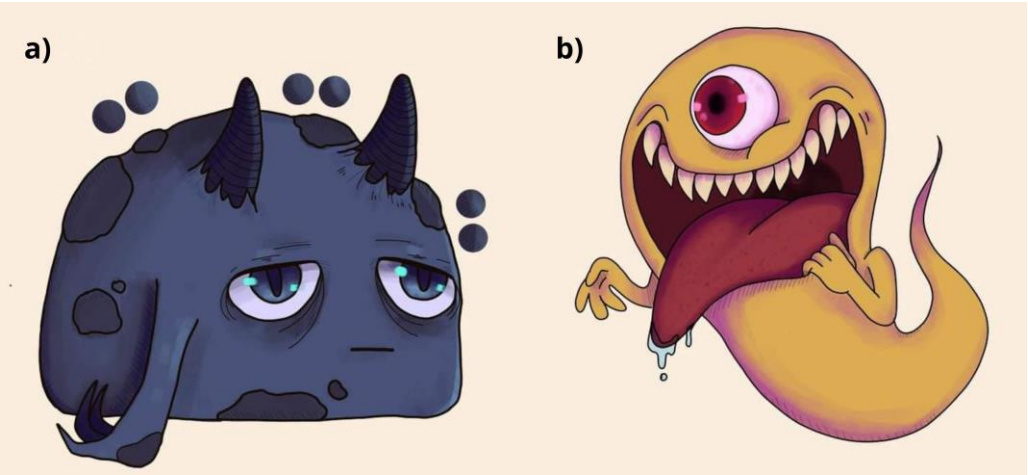


Figura 1: Monstros baseados em nucleófilo (a) e eletrófilo (b).

O NOVO REGIME CLIMÁTICO E A INTEGRAÇÃO DA EDUCAÇÃO AMBIENTAL CRÍTICA NA FORMAÇÃO DOCENTE INICIAL EM QUÍMICA E CIÊNCIAS BIOLÓGICAS.

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Palavras Chave:*educação ambiental crítica; formação de professores; mudanças climáticas; Bruno Latour*

Highlights

Mudanças climáticas e a formação docente inicial. Uma releitura da Educação Ambiental, compartilhando reflexões na perspectiva Discente~Docente~Aprendente.

Resumo/Abstract

O Novo Regime Climático desafia a sociedade a superar a visão modernista da separação entre natureza e sociedade. As mudanças climáticas (MC) aprofundam as desigualdades socioambientais, exigindo que a Educação Ambiental (EA) transcenda a vertente conservacionista, consolidada na formação docente brasileira com ações pontuais. Este trabalho apresenta resultados de uma pesquisa de mestrado que integrou a Educação Ambiental Crítica (EAC) de Carlos Frederico Bernardo Loureiro em diálogo com Bruno Latour. O objetivo foi fomentar repertórios teóricos e pedagógicos na formação inicial de professores de Ciências Biológicas na modalidade de Educação a Distância (EaD) e Química na modalidade presencial, ambos da Universidade Federal do Rio de Janeiro (UFRJ). O estudo destaca a importância de uma formação crítica para promover uma prática engajada com a justiça socioambiental. A metodologia fundamenta-se na perspectiva Discente~Docente~Aprendente (D~D~A)[1] envolvendo uma educação dialógica e afetiva por meio de tecituras com “c” e tessituras com “ss” visando multiplicar as experiênciações. Para os licenciandos de biologia implementou-se uma oficina remota no segundo semestre de 2024 associando conceitos químicos a EAC. Para os licenciandos em Química, realizaram-se três encontros no primeiro período de 2025, com rodas de conversa, produções imagéticas e narrativas discentes. Os resultados evidenciam que a integração da EAC ampliou a compreensão dos futuros docentes sobre a complexidade das MC. Conclui-se que a EAC na formação docente inicial fortalece a articulação entre ciência e sociedade, convergindo para uma reflexão sobre as raízes estruturais da crise ambiental.

[1]BARROS, S. C. R. et al. Inter-relações multi~ pluri~ inter~ trans~ indisciplinar (es) idade na perspectiva discente~ docente~ aprendente. Revista Scientiarum Historia, v. 1, n. 1, p. e510-e510, 2026.

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Ora-pro-nobis branches in the production of a mini-project for teaching adsorption: simplicity and efficiency in dye removal

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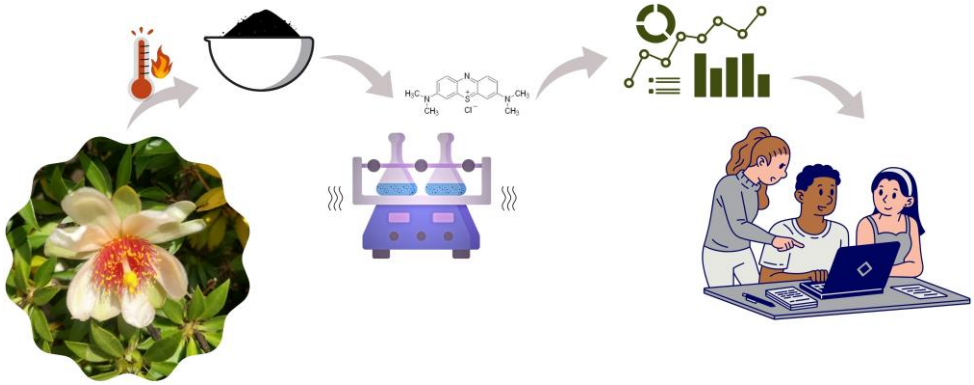
Palavras Chave:*Inquiry-Based Learning, Adsorption Teaching, Sustainable Chemistry Education, Biomass Valorization, Physical Chemistry*

Highlights

Inquiry-based mini-project to teach adsorption CURE approach in Physical Chemistry laboratory Sustainable biomass connects theory to practice Research skills and student engagement enhanced

Resumo/Abstract

This study presents the design and implementation of a five-week course-based undergraduate research mini-project aimed at teaching adsorption concepts within a Physical Chemistry II course for Agro-industrial Engineering students. Grounded in the principles of sustainability, inquiry-based learning, and Course-Based Undergraduate Research Experiences (CUREs), the project engaged students in the valorization of a locally available biomass, ora-pro-nobis (Pereskia aculeata Miller) branches, for the production of biochar adsorbents. Throughout the activity, students actively participated in all stages of the research process, including biomass processing and synthesis, interpretation of material characterization data (SEM, EDS, BET, FT-IR, and CHN), and evaluation of dye adsorption performance using batch experiments and UV-Vis spectrophotometry. Learning outcomes emphasized the development of experimental skills, learned material characterization techniques, critical interpretation of analytical data, hypothesis formulation, and scientific communication. Student-generated adsorption results showed high reproducibility when compared with control experiments, reinforcing the reliability of the experimental protocol and supporting student confidence in laboratory research. The mini-project also fostered collaboration, engagement, and motivation, as evidenced by student feedback and performance in seminars and written reports. By integrating authentic research practices with locally relevant and sustainable materials, this pedagogical approach effectively connected theoretical adsorption concepts to real-world environmental applications. The results demonstrate that research-oriented laboratory mini-projects represent a powerful strategy for enhancing conceptual understanding, scientific reasoning, and student agency in undergraduate chemistry education.



Ora-pro-nobis waste for teaching adsorption.

Agradecimentos/Acknowledgments

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Os desafios do ensino por projetos articulados aos ODS e a SNCT/2025 da 10° Feira de Ciências, Arte e Cultura do IFSP/MTO.

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Palavras Chave:*Ensino por projetos,Feiras de Ciências,ODS,SNCT,Popularização da Ciência*

Highlights

Feira de Ciências. Ensino por projetos como metodologia ativa. Desenvolvimento de projetos de IC/Jr com pelo menos um ODS e norteados pelo tema central da SNCT/2026.

Resumo/Abstract

As Feiras propiciam a popularização científica e são espaços favoráveis de atividades educativas e culturais que proporcionam elevada motivação à educação e à prática científica, pois oportunizam a criticidade, a criatividade, a colaboração, além de possibilitar a discussão de questões sociais. A metodologia seguida para atingir tais características foi o ensino por projetos, baseada no princípio de que, ao participar de um projeto, o aluno está envolvido em uma experiência em que o processo de construção de conhecimento está integrado às práticas vividas, desenvolvendo uma atividade complexa. Assim, pode-se afirmar que o objetivo geral foi o desenvolvimento de habilidades de pesquisa, sensibilização ambiental e a popularização científica, norteados pelo ensino por projetos, o tema central da 22° SNCT, “Planeta Água: a cultura oceânica para enfrentar as mudanças climáticas no meu território” e ODS. Ao todo, foram apresentados 41 trabalhos vinculados ao tema da SNCT, como exemplos, citamos: i. Mar que Nos Forma: ancestralidade africana e o sagrado das águas; ii. Salgado como o mar: o custo invisível do nosso consumo; iii. Energia que vem das ondas: o mar como fonte de futuro sustentável; iv. Biorremediação de áreas contaminadas com petróleo. Como resultados, pode-se citar o grande número de estudantes, mais de 2100, que visitaram a Feira, provindos de várias escolas públicas da cidade. O evento contou também com um grande número de familiares e comunidade em geral visitando as apresentações durante o período noturno. Pode-se afirmar que os estudantes e orientadores dedicaram-se de maneira exemplar no desenvolvimento dos projetos e que essa iniciativa oportunizou situações de aprendizado e, principalmente, reflexões sobre as responsabilidades que toda a população possui, mesmo estando há centenas de quilômetros de distância dos oceanos, sobre a cultura oceânica e o meio ambiente.

Agradecimentos/Acknowledgments

CNPq – Processo 421967/2025-0. IFSP/MTO

O vídeo educacional “Backdraft: o fogo e a química em ação” como recurso pedagógico para o ensino de Química

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Palavras Chave:*Ensino de Química,Combustão,Backdraft,Recursos Audiovisuais,incêndio*

Highlights

The use of the proposed educational video can enhance chemistry teaching by linking concepts of combustion, stoichiometry, and thermodynamics to the explosive backdraft phenomenon observed in fires.

Resumo/Abstract

Os conteúdos de combustão, termoquímica e estequiometria, embora fundamentais para a compreensão de processos naturais e tecnológicos, são frequentemente abordados no ensino médio de forma excessivamente teórica e descontextualizada, o que dificulta a aprendizagem dos estudantes. Nesse contexto, foi desenvolvido um vídeo educacional com o objetivo de articular teoria e prática por meio de uma linguagem acessível, sem prejuízo do rigor científico, tornando visíveis fenômenos de difícil experimentação em sala de aula. O vídeo “Backdraft: o fogo e a Química em ação” com duração de 4 min e 26 s (https://www.youtube.com/watch?v=BRQcFu7DGi4) integra imagens reais, animações explicativas e narração didática para abordar o fenômeno do*backdraft*, definido como uma explosão causada pela ignição súbita de gases combustíveis acumulados em um ambiente com deficiência de oxigênio, quando ocorre a entrada abrupta de ar durante um incêndio.

O desenvolvimento do recurso baseou-se em princípios pedagógicos alinhados à Base Nacional Comum Curricular (BNCC) e em referenciais sobre tecnologias educacionais e metodologias ativas. O vídeo foi concebido para promover a contextualização de conceitos químicos relacionados à combustão, à termoquímica e às relações estequiométricas, favorecendo a aprendizagem destes temas no ensino médio e o diálogo interdisciplinar entre Química, Física e Segurança Pública.

A aplicação do vídeo em turmas de escolas estaduais do Rio de Janeiro e de Minas Gerais, envolvendo 115 estudantes do ensino médio, indicou que o uso intencional do recurso audiovisual, associado à mediação pedagógica ativa e a práticas reflexivas, potencializou a aprendizagem. As discussões em sala evidenciaram maior engajamento, curiosidade e capacidade de relacionar conceitos químicos a situações do cotidiano, destacando o potencial do vídeo como ferramenta didática para o ensino de Química e para a formação cidadã.



Cena 6 do vídeo “Backdraft: o fogo e a Química em ação” ilustrando a combustão completa e incompleta

Agradecimentos/Acknowledgments

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Pedagogical Content Knowledge on Thermochemistry and Perspectives for Teacher Education in Graduate Programs

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Palavras Chave:*Teaching chemistry,Teacher education,PCK,Professional development*

Highlights

Possible pathways for teacher education of university-level chemistry instructors.
Integrative PCK and Transformative PCK.
Graduate education in teacher development beyond research training.

Resumo/Abstract

The construction of teaching knowledge should be an integral part of teacher education, including preparation for teaching in higher education. Pedagogical Content Knowledge (PCK) is one a key form of knowledge that enables teachers to make specific content teachable. It can be conceptualized through the integrative model, as the integration of pedagogical, content, and contextual knowledge, or through the transformative model, in which PCK, although related to these domains, is considered a distinct form of knowledge. This study discusses selected results from a master's/doctoral-level course designed to foster the development of PCK among graduate students at a public university in southern Brazil, based on the transformative model. The analysis focuses on responses from 11 participants, collected at the beginning and at the end of the semester, regarding thermochemistry content. During the course, participants discussed their initial ideas about key topics, became familiar with instructional strategies reported in the literature, engaged in pedagogical practice involving investigative cases (case-based learning), and reflected on epistemological aspects, contextual factors, and students' learning difficulties. By the end of the course, the responses showed a more homogeneous distribution across content topics and incorporated aspects that were initially absent or only marginally considered, such as the role of context, the laws of thermodynamics, Hess's law, and bond energy (Figure 1). These results indicate an expansion of participants' PCK components and the direct influence of the course on how they conceptualize the teaching of thermochemistry. The study reinforces the importance of graduate education in fostering pedagogical, contextual, and PCK-related knowledge, beyond research training, with a focus on university-level teaching.

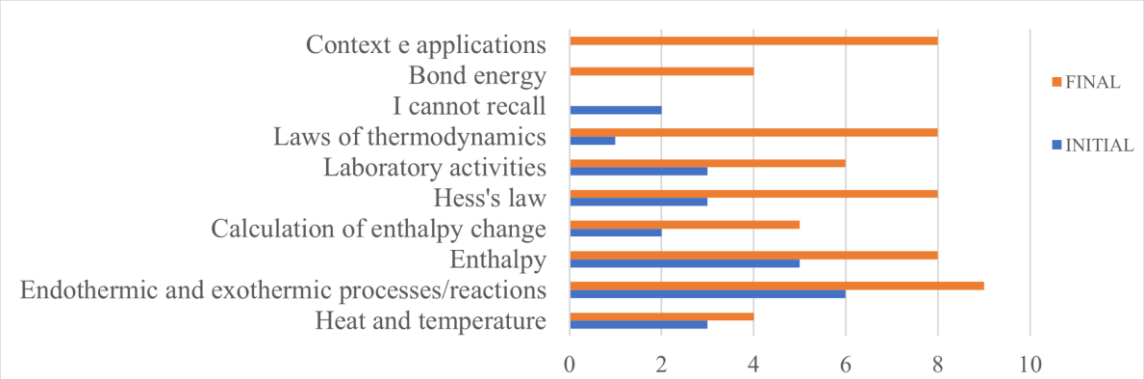


Figure 1 – Selected thermochemistry topics identified by the graduate students

Agradecimentos/Acknowledgments

The authors acknowledge the Universidade do Estado de Santa Catarina and the Fundação de Amparo à Pesquisa e Inovação do Estado de Santa Catarina (FAPESC).

pHIA: A Low Cost Application for pH Strip Analysis Using Artificial Intelligence.

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Palavras Chave:*pH, Accessibility, Application, Artificial Intelligence, Indicator Strips.*

Highlights

The pHIA project aims to promote greater accessibility and accuracy in pH measurement, particularly for individuals with visual impairments such as dyschromatopsia.

Resumo/Abstract

The determination of solution pH using pH meters, acid–base titrations, indicators, and colorimetric test strips constitutes a set of essential experiments in the education of high school and undergraduate students. However, such experimental practices are not accessible to everyone. Factors such as reduced visual acuity, aging, and conditions like dyschromatopsia may impair color perception, hindering the correct interpretation of results. In this context, the objective of this work was to develop a mobile application capable of enhancing both accessibility and accuracy in pH measurement, enabling users to perform analyses through their smartphone cameras. The application was developed for educational purposes by students of the Integrated Technical Course in Informatics at IFSP – Campinas Campus, as part of the requirements of the Integrative Project course. The cross-platform solution was built using React Native, allowing the capture of images of indicator strips and, with the support of predictive Artificial Intelligence (AI) models implemented in Python, the estimation of pH values. Measurements were performed using Macherey-Nagel indicator strips, while a digital pH meter was employed as a calibration reference, reducing variability and strengthening data reliability. In its first functional version, the pHIA application successfully captured images, analyzed them, and classified pH values in intervals of 1.5 units, eliminating the subjectivity inherent to human interpretation and providing a more accessible and reliable measurement. Nevertheless, further improvements are required. Future developments include refining the AI models, expanding the application's functionalities, implementing a database, increasing device compatibility with an emphasis on calibration across different mobile platforms, and incorporating additional colorimetric analyses.



Representation of the methodology used for the development of the pHIA mobile application.

Agradecimentos/Acknowledgments

Instituto Federal de Educação, Ciência e Tecnologia de São Paulo – Campus Campinas.

Por Dentro da Química – Segunda Temporada: A Tabela Periódica no Ensino de Química

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Palavras Chave:*Tabela Periódica; Ensino de Química; Podcast; Divulgação científica; Mídias digitais*

Highlights

Periodic table podcast series.
Chemistry education through digital media.
Connects elements to everyday life.
Accessible scientific communication.
Teacher training with podcasts.

Resumo/Abstract

A segunda temporada do podcast*Por Dentro da Química*teve como eixo central a Tabela Periódica, abordada como ferramenta fundamental para a compreensão da Química e de suas aplicações no cotidiano. Apresentado pelo Prof. Daltamir J. Maia e desenvolvido em parceria com a licencianda Letícia S. Ruzene, o projeto buscou promover a divulgação científica por meio de linguagem acessível e contextualizada, aproximando conceitos científicos do público.

Os episódios abordaram diferentes aspectos da Tabela Periódica, incluindo sua construção histórica, a organização em famílias e períodos, o processo de nomeação dos elementos, a essencialidade dos elementos químicos para a vida e a relação entre a origem estelar da matéria e a organização periódica. Esses temas permitiram discutir propriedades, classificações e aplicações dos elementos, favorecendo a contextualização do conhecimento químico.

A produção do podcast envolveu pesquisa, elaboração de roteiros, gravação e edição dos episódios, constituindo uma experiência formativa relevante para a licencianda. O processo exigiu a tradução de conceitos científicos para uma linguagem acessível ao público não especializado e favoreceu o desenvolvimento de habilidades de comunicação científica e uso de mídias digitais no ensino.

Estudos indicam que podcasts têm sido utilizados como ferramentas de comunicação científica e de aprendizagem, contribuindo para aproximar conteúdos especializados do público por meio de linguagem acessível e narrativa envolvente. Além disso, a produção de podcasts em contextos educacionais favorece o desenvolvimento de habilidades de comunicação científica e amplia o interesse por temas científicos (VAINIERI et al., 2023; MATTEWAL; SETHI, 2024; ZILZ; SCHUCK, 2026).

Assim, a experiência e a teoria indica a viabilidade do uso de podcasts como estratégia de divulgação científica e como recurso pedagógico complementar no ensino de Química, além de contribuir para a formação docente da licencianda.



Capa do podcast "Por Dentro da Química", projeto de divulgação científica do IFSP Campinas.

Agradecimentos/Acknowledgments

Agradecemos ao IFSP Campinas pelo apoio institucional e a todos os ouvintes que acompanham o podcast, contribuindo para o fortalecimento das ações de divulgação científica e educação em Química.

Projetos STEAM em uma disciplina universitária: evidências da mobilização do TPACK

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Palavras Chave:*TPACK,STEAM,formação inicial de professores,ensino de Química,projetos didáticos.*

Highlights

STEAM projects in initial teacher training.

STEAM experience and mobilization of teachers' interdisciplinary knowledge.

STEAM projects and TPACK development.

Resumo/Abstract

A formação inicial de professores de química para o uso de tecnologias digitais nos dias atuais continua sendo um desafio a ser enfrentado. Este estudo investiga como licenciandos em Química mobilizam componentes do TPACK (*Technological Pedagogical Content Knowledge*) no processo de elaboração de projetos STEAM (*Science, Technology, Engineering, Arts and Mathematics*) em uma disciplina de Tecnologias para o Ensino de Química. Participaram da investigação quatro licenciandos, que inicialmente vivenciaram uma prática-modelo sobre acidificação dos oceanos, fundamentada na abordagem STEAM, envolvendo experimentação investigativa e sensores digitais. Posteriormente, os licenciandos desenvolveram projetos STEAM sobre diferentes temáticas, os quais constituíram o principal corpus de análise. Os dados foram constituídos pelas propostas elaboradas pelos participantes, e a análise qualitativa, orientada pelo referencial do TPACK e pela análise de conteúdo, buscou identificar evidências de integração entre conhecimentos tecnológicos, pedagógicos e de conteúdo. Os resultados indicam que os licenciandos compreenderam a proposta STEAM e elaboraram projetos que integraram tecnologias digitais, estratégias investigativas e conteúdos químicos, evidenciando a mobilização dos componentes do TPACK. Observou-se o uso planejado de sensores e recursos digitais para a produção e interpretação de dados experimentais, aliado à construção de problemas investigativos contextualizados. Apesar de desafios relacionados à interdisciplinaridade, as propostas revelam avanços na articulação dos conhecimentos profissionais docentes. Conclui-se que o desenvolvimento de projetos autorais, apoiado por mediações reflexivas, constitui um caminho promissor para o fortalecimento do TPACK e da abordagem STEAM na formação inicial de professores de Química.

Agradecimentos/Acknowledgments

Agradece-se à Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) pelo apoio ao desenvolvimento desta pesquisa.

Prompt Engineering as a Pedagogical Strategy: Support from Generative Artificial Intelligence in the Construction of Graphs in Chemistry Education

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Palavras Chave:*Generative Artificial Intelligence, ChatGPT, Prompt Engineering, Chemistry Education, Graphical Representations.*

Highlights

Generative AI as support for chemistry teaching

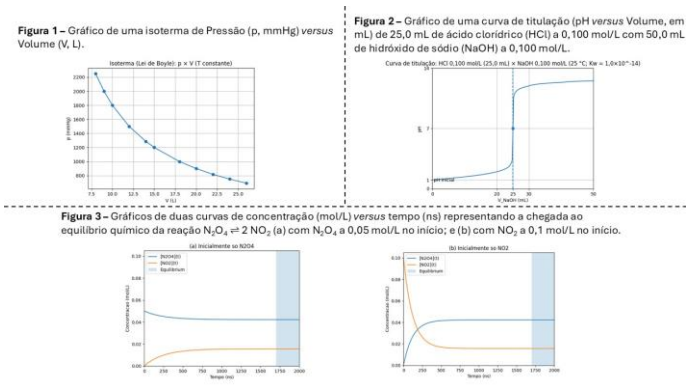
Prompt engineering applied to high school chemistry

Graph and question generation with pedagogy

Didactic consistency of ChatGPT outputs

Resumo/Abstract

Generative Artificial Intelligence (GAI) platforms, such as ChatGPT 5.2 Thinking, have emerged as yet another resource for teachers, provided that their use is guided by well-defined criteria. This study proposes Prompt Engineering (PE) strategies for Chemistry teachers, aimed at producing graphs for High School (HS) teaching, with outputs in JavaScript Object Notation (JSON). The methodology was structured in three stages: (1) selecting Chemistry topics; (2) designing and using prompts; and (3) conducting a Content Analysis of the responses obtained. In the first stage, we selected the following Chemistry topics: (i) chemical equilibrium, (ii) acid–base titration, and (iii) gas transformations. In the second stage, we designed prompts based on the following PE strategies: role-based prompting; use of delimiters; one-shot prompting; and iterative refinement. Starting from the initial prompt, we carried out successive interactions, arriving at a command capable of generating a graph and three High School-level questions for each topic. Finally, in the third stage, the graphs produced were analyzed and showed theoretical consistency when compared to those found in instructional materials for this educational level, and the interpretive questions proved applicable for classroom use. Thus, the results suggest that GAI, combined with PE strategies, can contribute to the pedagogical practice of Chemistry teachers. Below, we provide a link to access the respective interaction logs with ChatGPT: Interaction 1 – Obtaining a Pressure × Volume isotherm related to the topic of gas transformations (1st year of HS); Interaction 2 – Obtaining a titration curve for hydrochloric acid (HCl) with sodium hydroxide (NaOH) (2nd year of HS); and Interaction 3 – Obtaining two curves representing the approach to chemical equilibrium for the reaction N2O4 ⇌ 2 NO2 (2nd year of HS). Link: https://encurtador.com.br/aCsJ.



Graphs developed with the assistance of ChatGPT 5.2 Thinking using JSON.

Agradecimentos/Acknowledgments

This work was supported by the Coordination for the Improvement of Higher Education Personnel (CAPES), the São Paulo Research Foundation (FAPESP), and the Institute of Chemistry of the University of Campinas (UNICAMP).

Proposal of a tactile educacional material for the study of the greenhouse effect content for students with visual impairments in an inclusive context

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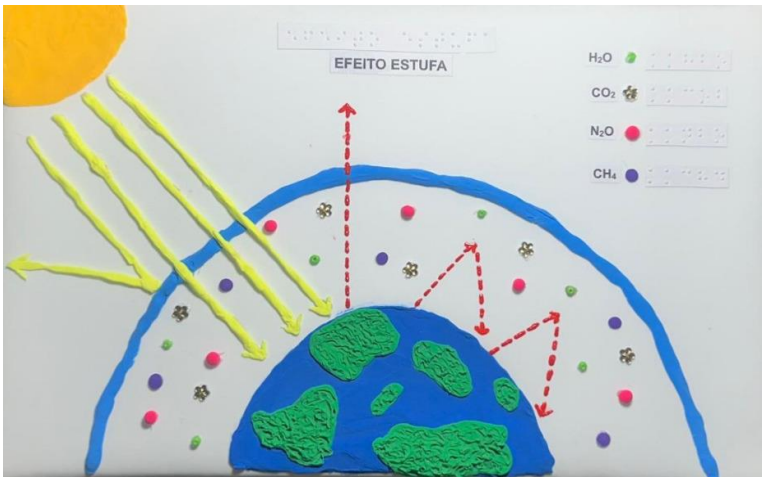
Palavras Chave:*Tactile Materials,Visual Impairments,Greenhouse Effect,Inclusive Education*

Highlights

A low-cost tactile model for the greenhouse effect was designed for chemistry classes, enabling students with visual impairment to grasp abstract concepts in inclusive classrooms.

Resumo/Abstract

Chemistry teaching often involves abstract concepts that are commonly presented through visual representations, which can limit access for students with visual impairment. The greenhouse effect, frequently explained through diagrams and images, exemplifies a concept whose understanding may be hindered for these students. Although the literature discusses inclusive education and accessibility in science teaching, few studies explore tactile resources specifically designed to support the teaching of the greenhouse effect in chemistry. This study aims to describe the development of a low-cost tactile model to support the teaching of the greenhouse effect in chemistry classrooms, allowing its replication by other teachers and contributing to more accessible science education. The model was designed based on textbook representations and on literature addressing tactile resources and inclusive practices in science education. A qualitative approach guided the study, including a bibliographic review conducted in the Brazilian Digital Library of Theses and Dissertations (BDTD), the CAPES Theses and Dissertations Catalog, the CAPES Journals Portal, and Google Scholar. The tactile material was built on a Styrofoam base with EVA components of different textures representing solar radiation, the Earth's surface, and greenhouse gases. A legend in Portuguese and Braille allows both visually impaired and sighted students to interpret the model.



Tactile representation of the greenhouse effect

Agradecimentos/Acknowledgments

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Protagonismo discente em Química via escape room: design, aplicação e decisão estratégica

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Palavras Chave:*Ensino de Química,Escape Room,Metodologias Ativas,BNCC*

Highlights

Immersive BNCC-aligned chemistry escape room boosts scientific literacy and decision-making; vertical station rotation enables large-class delivery (n=190) with rapid teacher code validation.

Resumo/Abstract

A Base Nacional Comum Curricular (BNCC) propõe que o ensino de Química desenvolva o letramento científico e a capacidade de tomar decisões frente a desafios contemporâneos (Brasil, 2018). Nesse panorama, os jogos educacionais têm sido discutidos como estratégias promissoras para potencializar o engajamento e a participação ativa do estudante.

Esse trabalho relata a aplicação de um escape room fundamentado em uma narrativa imersiva, no qual o estudante assume o protagonismo na resolução dos enigmas. O design pedagógico foi estruturado conforme o modelo de Cleophas e Cavalcanti (2020), inserindo os discentes em um cenário cujo a missão é posicionar o país como líder global na produção de baterias para veículos elétricos.

A intervenção envolveu 190 alunos do Ensino Médio com idade entre 15 e 16 anos e consistiu na resolução de quatro enigmas sequenciais que integraram conteúdos sobre Tabela Periódica, Separação de Misturas e Estequiometria. A dinâmica empregou uma adaptação da Rotação por Estações em formato vertical, viabilizando a aplicação em turmas numerosas.

Os resultados, coletados via questionário de autorrelato em escala Likert, indicaram elevado engajamento e percepção positiva de autonomia: 83% dos participantes classificaram a atividade como plenamente divertida e 93% (entre respostas totais e parciais) reconheceram que puderam escolher as estratégias de resolução. Os achados evidenciam que o design de escape room atua como um catalisador para a apropriação conceitual e o fortalecimento da autonomia discente. A eficácia demonstrada posiciona esta estratégia como uma alternativa metodológica replicável. Conclui-se que a intervenção cumpre as diretrizes de protagonismo da BNCC e oferece um modelo de atividade engajadora e pedagogicamente intencional.

Agradecimentos/Acknowledgments

Agradeço ao PROFQUI e à UNESP Araraquara – Instituto de Química pelo apoio à formação docente e às condições acadêmicas que viabilizaram este estudo.

QUALIDADE DO AR E FROTA VEICULAR EM REGIÕES METROPOLITANAS: UMA PROPOSTA DE JOGO DE TABULEIRO PARA O ENSINO DE QUÍMICA

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Palavras Chave:*ludicidade; material particulado; divulgação científica; educação ambiental crítica; ozônio*

Highlights

Compartilhando experiências da iniciação científica na perspectiva Discente~Docente~Aprendente. Proposta de jogo educativo para elaborar estratégias de controle de formação de ozônio troposférico.

Resumo/Abstract

Segundo a Organização Mundial da Saúde (OMS), o ozônio é um dos principais poluentes atmosféricos, causando danos à saúde pública, à fauna e à flora. O ozônio é formado a partir de precursores como os hidrocarbonetos não metano (HCNM) emitidos por veículos automotores. Assim, conhecer a contribuição de veículos e dos tipos de combustíveis para a emissão de HCNM é essencial para o controle da formação de ozônio nas grandes cidades. Este trabalho vinculado à iniciação científica (IC) propõe um jogo de tabuleiro para a divulgação científica, sobre o monitoramento da qualidade do ar nos municípios do Rio de Janeiro e Niterói. O objetivo foi desenvolver uma atividade lúdica para alunos do segundo ano do ensino médio, visando difundir o trabalho desenvolvido na IC sobre as emissões de material particulado (MP) e HCNM pela frota veicular. A metodologia baseia-se na abordagem Discente~Docente~Aprendente (D~D~A)[1], empregando diálogos colaborativos construídos ao longo das atividades de IC, que subsidiaram o planejamento da atividade lúdica. O jogo é estruturado para dois participantes, onde cada aluno assume a gestão ambiental de uma cidade distinta (Rio de Janeiro ou Niterói). O funcionamento exige que os participantes pensem em estratégias para mitigar a formação do ozônio, associando as classes de veículos, tipos de combustíveis e idade da frota, de modo a reduzir as fichas de poluentes HCNM e MP. O resultado alcançado foi a elaboração do jogo fundamentado na abordagem D~D~A[1], o que possibilitou ao aluno de IC transpor conteúdos técnicos e vivenciar um processo formativo que consolidou seu aprendizado por meio da popularização desses saberes. O material contribui para que os estudantes reflitam sobre o planejamento das cidades sob o viés da Educação Ambiental Crítica (EAC).

[1]BARROS, S. C. R. et al. Inter-relações multi~ pluri~ inter~ trans~ indisciplinar (es) idade na perspectiva discente~ docente~ aprendente. Revista Scientiarum Historia, v. 1, n. 1, p. e510-e510, 2026.

Agradecimentos/Acknowledgments

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Química do Consumidor Consciente: Uma proposta de oficina temática

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Palavras Chave:*consumidor consciente, oficina temática, alimentação*

Highlights

Chemistry of conscious consumer: a proposal of thematic workshop is an assignment suggestion of an approach between chemistry and a healthy diet for high school students.

Resumo/Abstract

O avanço da tecnologia e das mídias digitais, nos últimos anos, provocou uma onda de desinformação em diversas áreas do conhecimento, como a alimentação. As divulgações sensacionalistas, feitas por pessoas não necessariamente habilitadas em nutrição ou áreas afins, de ideias relacionadas ao bem-estar, levam muitas pessoas a adotarem hábitos de consumo sem verificar sua procedência e eficácia, afetando muitos jovens, um dos principais públicos das redes sociais (Guimarães; Cordeiro, 2024). A partir disso, discutiu-se a necessidade de fomentar o pensamento crítico dos estudantes sobre alimentação.

Uma oficina temática para alunos do ensino básico com o título “Química do Consumidor Consciente” foi desenvolvida a fim de discutir e estimular a reflexão sobre alimentação. Essa atividade consiste em uma sequência de experimentos de caráter investigativo, nos quais grupos de alunos realizam práticas experimentais para entender uma determinada ideia e como aquilo se relaciona com o seu cotidiano (Marcondes, 2008). A oficina contém 4 experimentos, são eles: condutibilidade dos alimentos, teste de ferro em leite e farinha, queima de alimentos e composição de refrigerantes.

Após a atividade, os alunos respondem um formulário de avaliação da oficina, relatando sua experiência e sua contribuição para a vida. Destacamos aqui algumas observações dos dados coletados, os alunos demonstram gostar da oficina e desejam participar mais vezes. Além de afirmarem aprender mais sobre química com as discussões, mais de 60% dos estudantes declaram que após as atividades são capazes de tomar decisões que implicam em uma alimentação mais saudável e consciente. No entanto, essa mudança não é trivial e se mostra desafiadora para outra parte dos participantes. Assim, é possível concluir que atividades como essa são relevantes para a formação do aluno como cidadão.

GUIMARÃES, T.; CORDEIRO, R. I. Em Questão, v. 30, p. e-138528, 2024.

MARCONDES, M. E. R. Revista em extensão, v. 7, n. 1, p. 67-77, 2008.

Agradecimentos/Acknowledgments

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Química Verde em exposição: repensando a vida de forma sustentável no Centro de Ciências de Araraquara (CCA)

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Palavras Chave:*Processo curatorial,Química Verde,Museu de ciências*

Highlights

Interactive exhibition focused on Green Chemistry principles in a science museum context.

Resumo/Abstract

A Química Verde (QV) tem como objetivo tornar a química mais segura por meio da prevenção[1], nesse contexto, se destaca como uma importante aliada para contribuir em um futuro mais consciente, equilibrado e responsável ao promover práticas mais sustentáveis.

O Centro de Ciências de Araraquara (CCA) é um museu vinculado UNESP de Araraquara e tem um papel importante na comunidade, especialmente na divulgação científica. Dessa forma, através do programa Conexões Museus SP, houve um processo de curadoria compartilhada entre o Museu Catavento e o CCA para a criação da exposição “Química Verde: repensando a vida de forma sustentável”.

O processo curatorial se iniciou em agosto de 2025, em que as equipes dos dois museus pesquisaram e criaram toda a concepção expográfica da exposição. A exposição é interativa, portanto, além dos painéis expositivos, foram elaborados jogos didáticos e um experimento.

A exposição possui uma dinâmica em que pode ser usada em visitas mediadas ou autoguiadas. O acervo conta com totens informativos e materiais interativos como um jogo da memória sobre os 12 princípios da QV. Nas visitas mediadas, há uma parte experimental do experimento “relógio de iodo” adaptado com a QV e um jogo de perguntas e respostas dos 12 princípios, que pode ser realizado e adaptado de acordo com os visitantes.

Durante a inauguração da exposição, realizada em 9 de fevereiro de 2026, cerca de 43 visitantes participaram da atividade, tendo a oportunidade de conhecer a exposição e vivenciar sua dinâmica.

Esta exposição propõe uma nova concepção para a apresentação da química em museus de ciência ao integrar experimentos, painéis expositivos e jogos, além de destacar a importância de parcerias entre museus e dar visibilidade à QV, promovendo a reflexão dos visitantes sobre a relação entre a química, os seres humanos e o meio ambiente.

[1] Anastas, P. T.; Warner, J. C.*Green Chemistry: Theory and Practice*. Oxford: Oxford University Press, 1998.



Sala da exposição "Química Verde: repensando a vida de forma sustentável".

Agradecimentos/Acknowledgments

Agradecimentos ao Museu Catavento, Programa Conexões Museus- SP, SISEM- SP, COPE-UNESP e IQ-UNESP.

Radiochemistry in the interdisciplinary context for analytical, inorganic, organic, and medicinal chemistry, focusing on cancer diagnosis and therapy

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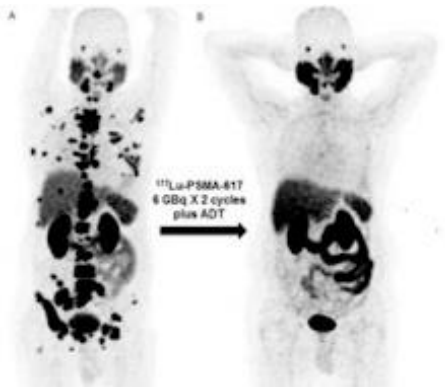
Palavras Chave:*Radiochemistry,Interdisciplinarity,Cancer,Therapy,Radioisotopes*

Highlights

Since Marie Curie´s time, chemistry has played a fundamental role in the development of radiochemistry and its use in medicine. Thus, radiochemistry should be included in the chemistry curriculum.

Resumo/Abstract

Marie Curie utilized her expertise in classical analytical chemistry to successfully separate and identify radioactive elements such as radium and polonium. Following her pioneering work, other researchers began to analyze samples of various minerals, employing foundational techniques in radioanalytical chemistry, since alpha (α) and beta (β) emissions were already recognized and identifiable. These investigations revealed that certain samples produced distinct radioactive compounds through decay chains, establishing the radioactive series ^{238}U, ^{235}U, and ^{232}Th. It was through these studies that Frederick Soddy recognized that some elements shared identical chemical properties but exhibited different radioactive behaviors, ultimately defining the concept of isotopes—elements occupying the same (iso) position (topic) in the periodic table. In the early 20th century, chemist George de Hevesy explored the use of elements from radioactive series in plants and animals, paving the way for what is now known as nuclear medicine. With the advent of particle accelerators and nuclear reactors, the availability of radioisotopes skyrocketed to thousands, with several dozen now used in medical applications. Noteworthy diagnostic agents include ^{18}F, as well as the radiometals ^{64}Cu, ^{68}Ga, and ^{99}mTc. In cancer therapy, β-emitting isotopes such as ^{90}Y, ^{153}Sm, and ^{177}Lu are used, alongside α-emitting isotopes such as ^{223}Ra, ^{225}Ac, and ^{211}At. While analytical chemistry remains vital, the fields of organic and inorganic synthesis of coordination compounds also play significant roles in developing molecules for cancer diagnosis and treatment. Furthermore, medicinal chemistry is crucial for creating molecules that target specific molecular targets in the cellular and tumor microenvironment. This underscores the necessity of including radiochemistry as an optional discipline in undergraduate chemistry curricula, reflecting its interdisciplinary nature.



177Lu-PSMA-617 Radioligand Therapy in Metastatic Prostate Cancer. Eur Urol 80, 390-392, 2021.

Agradecimentos/Acknowledgments

CEPID CancerThera - Grant FAPESP 2021/10265-8; INCT-PICS - Grants CNPq 408417/2024-2, Capes 88887.197686/20, FAPESP 2025/26818-7.

RELATO DA IMPLEMENTAÇÃO DE UM JOGO PEDAGÓGICO COMO ESTRATÉGIA PARA A EDUCAÇÃO ALIMENTAR

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Palavras Chave:*eduacação alimentar,química dos alimentos,jogo pedagógico,trabalho em grupo,inclusão*

Highlights

Atividades lúdicas tornam os conteúdos ministrados mais prazerosos e significativos

A alimentação saudável trabalhada de forma integrada aos conhecimentos dos nutrientes e os efeitos sobre a saúde

Resumo/Abstract

O ensino sobre alimentação tem ganhado cada vez mais relevância, já que a educação alimentar contribui para o desenvolvimento de competências que permitem aos alunos compreender a importância da escolha consciente dos alimentos, relacionando composição química dos mesmos, nutrição, saúde e bem-estar. Paralelamente, a gamificação, entendida como o uso de mecânicas de jogos em contextos educativos, contribui para aumentar a motivação intrínseca e o sentimento de progresso dos estudantes.[1] As oficinas pedagógicas também se configuram como estratégias relevantes, favorecendo o trabalho colaborativo, a criatividade e a aprendizagem.

Este trabalho investiga o uso de um jogo como ferramenta pedagógica para promover a educação alimentar e nutricional no Ensino Fundamental. O objetivo foi avaliar como metodologias lúdicas podem estimular o aprendizado sobre alimentação saudável de maneira interativa e inclusiva. Foi criado um jogo pedagógico adaptado sobre grupos alimentares na pirâmide alimentar. A atividade foi aplicada com 45 crianças de 11 a 13 anos do 6º ao 8º ano. O jogo é composto por um tabuleiro, peões, um dado numerado, e cartas de boas práticas e de maus hábitos e cartas com os nutrientes. Cada jogador, ao lançar o dado, avança no tabuleiro e coleta cartas de nutrientes correspondentes ao alimento sorteado. O objetivo é preencher corretamente a pirâmide alimentar individual, distribuindo os nutrientes nos grupos adequados: carboidratos, lipídios, laticínios, proteínas e vitaminas.

O uso do jogo aumentou o engajamento e facilitou a compreensão dos conceitos abordados na aula, promovendo também a cooperação e o desenvolvimento social. Conclui-se que a adoção de jogos analógicos constitui uma prática pedagógica dinâmica, acessível e inclusiva, que estimula a socialização, a troca de idéias e a criatividade e que poderia ser aplicada com sucesso em outras temáticas na área de ciências.

Referência

1- Oliveira e Ramos, 2021. https://doi.org/10.5585/eccos.n56.11199

Agradecimentos/Acknowledgments

Os autores agradecem ao Curso de Especialização Docente em Ciências (UFRJ) e o financiamento parcial do CNPq.

Relato da oficina “Química em chamas o poder da combustão, usando o lixo para cuidar da água” aplicada para estudantes da Educação Básica

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Palavras Chave:*Popularização da ciência,Ensino de Química; Letramento científico; Fotocatálise heterogênea; Extensão universitária; Pesquisa científica*

Highlights

Experimental workshop on photocatalyst synthesis using biomass. Photocatalysis application with active participation of high school students and teachers. Student motivation and scientific literacy.

Resumo/Abstract

As atividades de ensino, pesquisa e extensão desenvolvidas de forma integrada pelas universidades são fundamentais para a disseminação do conhecimento científico na sociedade. Ações realizadas em parceria com professores e estudantes da educação básica (feiras, oficinas...) contribuem para a alfabetização científica e para a formação de discentes críticos, aliados no enfrentamento do negacionismo. Assim, o Grupo de Estudos em Materiais e Catálise da UNEB, em colaboração com docentes do curso de Licenciatura em Química, vem promovendo ações de interação com a Rede Estadual de Ensino da Bahia. Em novembro de 2025, foi realizada uma oficina com duração de três horas envolvendo a síntese por combustão de um fotocatalisador à base de óxido de ferro obtido a partir de resíduo da agroindústria, bem como sua aplicação na fotocatálise do azul de metileno. Participaram da atividade 33 estudantes e 3 professores do Ensino Médio. Os experimentos foram precedidos por explicações teóricas ministradas por discentes de mestrado e de iniciação científica, responsáveis pela condução da atividade. A participação dos estudantes da educação básica foi ativa: seguindo um roteiro previamente elaborado, realizaram etapas experimentais como tomada de alíquotas, aferição de balões volumétricos, leituras em espectrofotômetro e uso de balança analítica. Durante a oficina, os participantes demonstraram compreensão dos conceitos abordados, evidenciada por perguntas e comentários relacionados à síntese, ao reaproveitamento de resíduos e à fotocatálise. Também houve interesse pela trajetória acadêmica dos estudantes envolvidos. Segundo relato de um dos professores acompanhantes, a experiência estimulou reflexões sobre o futuro acadêmico e profissional dos alunos, levando alguns a considerar o ingresso no curso de Licenciatura em Química. Conclui-se que a oficina contribuiu para a motivação dos estudantes e para o letramento científico, ao proporcionar vivências das atividades-fim da universidade.

Agradecimentos/Acknowledgments

Ao Programa de Pós-graduação em Química Aplicada e ao Curso de Licenciatura em Química do DCET-I/UNEB. Ao PIBIC-CNPq pelas bolsas concedidas. Ao Colégio Estadual Centro Territorial de Educação Profissional da Região Metropolitana.

Specialty Coffee Roasting and Its Effects on Human Health: A Natural Phenomenon of Educational Value for Chemistry Education

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Palavras Chave:*Torra café especial,saúde humana,fenômeno natural com valor educativo,Educação Química,Specialty Coffee Roasting*

Highlights

Specialty coffee roasting is scientifically relevant natural phenomenon with educational value for chemistry education.

Resumo/Abstract

O café é uma bebida muito consumida no mundo e pode causar efeitos na saúde humana (Mkiso et al., 2024). Considerando tais efeitos, o objetivo é analisar se os efeitos da torra do café especial para a saúde humana podem ser caracterizados como um fenômeno com valor educativo para o ensino de Química. Portanto, buscamos responder se esse fenômeno apresenta critérios que determinam seu valor educativo. Metodologicamente, realizou-se uma análise teórico-conceitual baseada em literatura científica sobre os processos físico-químicos envolvidos na torra do café e sobre os efeitos das substâncias formadas no organismo humano, após a ingestão da bebida. A análise foi organizada a partir de quatro dimensões: contextual, científica, cognitiva e social (Pereira et al., 2026). Na análise consideram-se os processos físico-químicos da torra e a influência das substâncias produzidas no organismo humano, dada a ingestão da bebida. Considera-se fenômeno com valor educativo aquele que apresenta as dimensões citadas para sua explicação. Os resultados indicam que o fenômeno pode ser compreendido a partir da articulação entre os processos físico-químicos da torra e bioquímico-fisiológicos relacionados à interação da bebida com o corpo humano. Essa interpretação requer uma articulação interdisciplinar de diferentes campos de conhecimento, caracterizando-o como fenômeno complexo em que se pode adotar a modelização como perspectiva de ensino. Portanto, os efeitos da torra para a saúde humana apresentam dimensões que justificam seu valor educativo, uma vez que se trata de efeitos com probabilidade de ocorrência na população brasileira devido ao consumo da bebida. Este fator também pode justificar a dimensão social, pois o consumo pode trazer benefícios e malefícios à saúde humana. Desse modo, o efeito para a saúde humana do consumo de uma bebida cuja torra determina as substâncias a serem produzidas foi considerado de valor educativo, podendo ser incorporado ao ensino de Química.

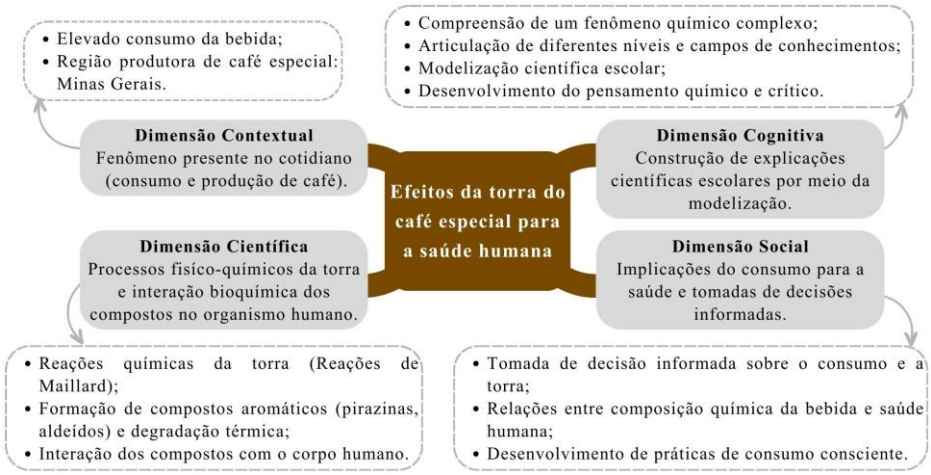


Figura 1. Interação entre dimensões conceituais justificando interesse científico e valor educativo

Agradecimentos/Acknowledgments

Apoio CAPES, FAPEMIG, UNIFAL-MG.

Specialty Coffee Roasting: Proposal of a Scientific Model for Chemistry Education

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Palavras Chave:*Torra de café,café de especialidade,modelização científica,ensino de química*

Highlights

Specialty coffee roasting involves physical and chemical transformations that shape sensory attributes. In higher education, understanding this process requires scientific models.

Resumo/Abstract

Minas Gerais ocupa uma posição destacada na produção de cafés de especialidade no Brasil. A torra do café determina características sensoriais e a composição de substâncias voláteis e não voláteis (Alcantara, 2025). Ao considerar a educação superior, a modelização científica do processo de torra favorece a compreensão dos processos químicos de um fenômeno de relevância social, econômica e científica, que apresenta valor educativo. O objetivo deste estudo é apresentar e discutir um modelo científico com valor educacional para ensino superior de química sobre a torra do café de especialidade. Para isso, realizou-se uma revisão sistemática que buscou descrever os processos e as reações químicas envolvidas. A busca foi realizada nas bases ScienceDirect, Scopus e Google Scholar, utilizando descritores em português, inglês e espanhol, sendo eles: “processo de torra” AND “café” AND “café arábica” AND “Reação de Maillard” AND “ Química”. Foram analisados estudos publicados nos últimos cinco anos. O resultado consiste em um modelo com duas dimensões: a ontológica — entidades e suas propriedades — e a epistemológica — relações de causa e efeito e inferências (López y Mota, 2019). Sob determinadas condições de temperatura e tempo, as entidades químicas que compõem o grão participam de transformações, como as reações de Maillard e a caramelização, que contribuem para o escurecimento. Em uma das etapas, a glicina interage com açúcares redutores, formando compostos instáveis, as glicosaminas, que se reorganizam em cetoaminas e, por reações adicionais, produzem compostos aromáticos sensoriais, polímeros nitrogenados e melanoidinas (Lee; Choi; Lee, 2024). O valor educativo do modelo pode ser atribuído a compreensão de um fenômeno complexo, a explicação causal, permitindo relacionar as propriedades para inferir sobre possíveis efeitos, articulação de diferentes níveis de representação do conhecimento químico e desenvolvimento do pensamento químico científico.

Agradecimentos/Acknowledgments

Apoio CAPES, FAPEMIG (APQ 00544-23/APQ-05218-23), UNIFAL-MG, UPN-Ajusco.

Sustentabilidade e poluição de solos: uma análise da produção de atividades de professores de Química em uma ação de formação continuada

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Palavras Chave:*sustentabilidade,abordagem CTSA,ensino de química,solos,poluição,ensino de Química*

Highlights

Chemistry teachers shared ideas about sustainability related to environmental issues, neglecting the economic ones. These results emphasize the need of training to foster social and economic literacy.

Resumo/Abstract

Neste trabalho, analisamos como professores de Química planejam atividades sobre o tema solo, considerando aspectos relativos à sustentabilidade e à poluição, investigando suas visões e práticas sobre a contextualização social de conteúdos de Química, em uma perspectiva de ensino CTSA.
A coleta de dados ocorreu em um curso de 30 horas, presenciais, no qual participaram 22 professores de Química do ensino médio de escolas públicas de São Paulo que formaram 4 grupos, dois deles desenvolvendo o tema solo. A ideia de sustentabilidade desses professores está, geralmente, associada a questões ambientais, sem considerar outros aspectos importantes, conforme indica a análise do instrumento em que os professores manifestaram ideias relativas à abordagem da sustentabilidade no ensino de Química. Nessa análise, verificamos que 70% dos professores concordam plenamente com a abordagem nas aulas de Química de aspectos ambientais e sociais, mas 30% deles discordam que questões econômicas devam ser tratadas no ensino. Entretanto, Sachs (2002) aponta que uma das dimensões da sustentabilidade é a econômica, envolvendo o gerenciamento mais eficiente de recursos, considerando não apenas a rentabilidade, mas também aspectos sociais. Sachs (2002, p. 85-89) propõe 8 dimensões para a sustentabilidade: a ecológica, a social, a cultural, a ambiental, a econômica, a territorial, a política (nacional) e a política (internacional). O material produzido por dois grupos de professores focou o tema agrotóxico, reforçando a sustentabilidade ambiental e sua relação com conteúdos químicos.
Os resultados sugerem a necessidade de ações formativas que enfoquem o ensino de Química e a sustentabilidade considerando, também, aspectos econômicos e sociais, produzindo materiais para a compreensão dos alunos sobre o significado de sustentabilidade e a responsabilidade individual e coletiva ao tomar decisões sobre situações cotidianas.

SACHS, I. Caminhos para o Desenvolvimento Sustentável. RJ: Garamond, 2002

Agradecimentos/Acknowledgments

Ao Instituto de Química da USP e ao professores participantes do curso de formação continuada.

SwiperPy: Atomic Orbital Generator for 3D Printing

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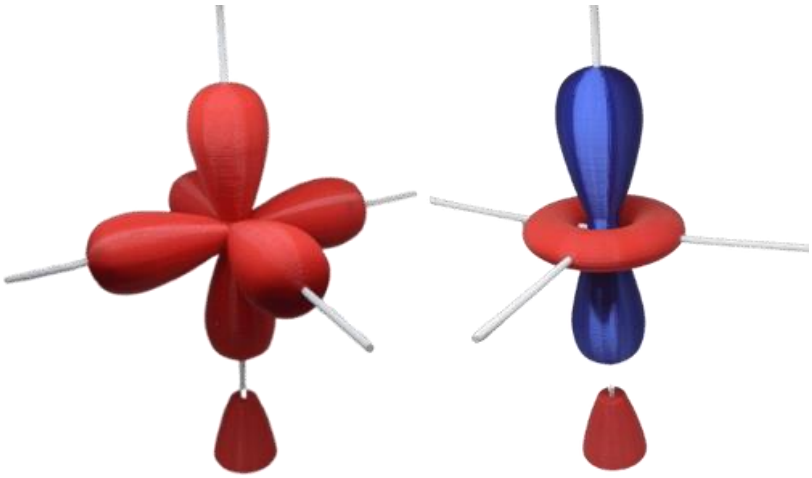
Palavras Chave:*Orbitals,3D Printing,Educational,Inclusion,Objects*

Highlights

3D printing in chemistry; Inclusion in chemistry; Python programming; Molecular orbital models in tactile and visual formats.

Resumo/Abstract

Over the last decade, 3D printing has grown in popularity in various fields, from medicine to aerospace engineering. In academic circles, this technique has been adopted for research and educational purposes, where the objects thus produced have been shown to facilitate the design of experiments, and the teaching- learning relationship, as well as promote the creative process. The integration of 3D printing in chemistry classrooms and other scientific and engineering disciplines has shown beneficial effects, as it facilitates the understanding and interpretation of abstract concepts associated with the description of electronic structure through atomic and/or molecular orbital models in tactile and visual formats. In this work, an open-source Python program called SwiperPy was developed to generate models of atomic orbitals and the necessary files required for 3D printing it. The orbitals are built by normalized linear combinations of spherical harmonics that resolve the non-time dependent Schrödinger equation in spherical coordinates. The objects obtained are then discretized in order to generate the STL files using triangulation of surfaces. SwiperPy is a user-oriented program that facilitates the construction of atomic orbitals by entering a few arguments in the command line or selecting from a list. This program can be used on a local computer or in web-based platforms, and can be obtained for use and/or modify from https://github.com/Hapuqs/IC. In addition to producing teaching resources that explain the orbitals concept, this project promotes inclusion in the educational environments. The tactile nature of the objects significantly helps students with visual impairments or cognitive deficits.



3D Representation of a Spherical Harmonic and a Atomic Orbital

Agradecimentos/Acknowledgments

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Tabela Periódica On-line Colaborativa: Vinte Elementos QuímicosAplicados à Saúde

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Palavras Chave:*Tabela Periódica,Aplicação na área da saúde,Padlet,aprendizagem colaborativa,ferramentas digitais*

Highlights

An online, collaborative Periodic Table built with Padlet to improve chemistry learning. It connects chemical elements to health applications, boosting student engagement and contextual understanding.

Resumo/Abstract

Este resumo apresenta o desenvolvimento e a aplicação da "Tabela Periódica da Saúde", um produto educacional construído na plataforma digital Padlet. A proposta trata do desafio de superar a abordagem tradicional e abstrata do ensino da Tabela Periódica, conectando elementos químicos a aplicações práticas e altamente relevantes para estudantes do Ensino Médio, com foco na saúde humana. A ferramenta utiliza uma interface multimodal, integrando textos, imagens e podcasts, e destaca-se pela sua natureza colaborativa, permitindo que estudantes e professores participem ativamente na construção do conhecimento. A aplicação da ferramenta em turmas do Ensino Médio e Educação de Jovens e Adultos (EJA) demonstrou um aumento significativo no engajamento discente e uma maior apropriação de conceitos químicos, validando a metodologia como uma alternativa eficaz para um ensino de Química mais dinâmico, significativo e alinhado com as demandas da educação contemporânea.

Agradecimentos/Acknowledgments

Os autores agradecem ao PROFQUI, à CAPES pelo fomento e à Universidade Federal do Rio de Janeiro (UFRJ) pelo apoio institucional.

TABELAR: UM JOGO DIDÁTICO PARA O ENSINO DE PROPRIEDADES PERIÓDICAS E QUÍMICA INORGÂNICA

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Palavras Chave:*tabela periódica,química inorgânica,baralho*

Highlights

A game using the periodic table and riddle-based cards on elemental properties enhances conceptual understanding and connects chemistry content to real-world applications through active learning

Resumo/Abstract

O ensino de Química, especialmente de Química Inorgânica e da Tabela Periódica, apresenta desafios relacionados ao caráter abstrato dos conteúdos e à dificuldade de estabelecer conexões entre propriedades dos elementos e suas aplicações. Nesse contexto, este trabalho descreve a aplicação do jogo didático Tabelar em uma turma do Ensino Médio do IFCE – Campus Aracati, composta por 26 estudantes, com o objetivo de favorecer a aprendizagem dos elementos químicos e de suas propriedades por meio de uma abordagem interativa e colaborativa. O recurso consiste em uma tabela periódica em lona (99,6 × 69,6 cm), fichas magnéticas numeradas e um baralho de cartas contendo charadas relacionadas a propriedades e características dos elementos químicos, como número atômico, grupo e período, classificação, propriedades periódicas, reatividade química e aplicações no cotidiano. A dinâmica ocorre em equipes, que participam de rodadas nas quais devem identificar corretamente os elementos a partir das pistas apresentadas, mobilizando conhecimentos sobre suas propriedades e posição na Tabela Periódica. Após a aplicação, foi utilizado um questionário avaliativo em escala Likert. Os resultados indicaram elevada aceitação da atividade: 80,8% dos estudantes concordaram totalmente que o jogo tornou as aulas mais dinâmicas e interessantes, enquanto 92,3% relataram melhora na compreensão dos conteúdos, sendo 50% em concordância total. Além disso, 69,2% recomendariam o jogo a outros alunos com concordância total, 84,6% avaliaram positivamente o trabalho em grupo e 92,3% consideraram as instruções iniciais suficientes. Os resultados sugerem que a utilização do jogo favorece o engajamento e a cooperação entre os estudantes, além de estimular a aprendizagem conceitual ao promover a discussão e a identificação de propriedades e características dos elementos químicos durante a resolução das charadas, sendo uma estratégia pedagógica eficaz e motivadora para o ensino de Química Inorgânica.



FIgura 1. Cartas do jogo Tabelar

Agradecimentos/Acknowledgments

IFCE – Campus Aracati

PIBID – Sub-projeto Química – IFCE – campus Aracati

CAPES

Tactile Didactic Boards as an Assistive Technology Resource in Chemistry Education for Students with Visual Impairments

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Palavras Chave:*Assistive Technology,Chemistry Education,Visual Impairment,Tactile Learning Materials,Inclusive Education*

Highlights

Integration of Assistive Technology tools such as Braille printing, thermal relief printing, 3D printing. Contribution to accessible and inclusive Chemistry teaching practices in university settings.

Resumo/Abstract

The inclusion of students with disabilities in Chemistry education requires the adoption of pedagogical practices that promote autonomy and active participation in the learning process. Therefore, this study aimed to develop Tactile Learning Boards for use by visually impaired students (blind and low vision) in the Fundamentals of Chemistry course at the Federal University of Recôncavo da Bahia. The research was structured in three stages: selection of essential topics covered in the course content; adaptation of the content and images (graphs, figures) using the free software Braille Fácil and Monet; and printing using a Braille printer, a thermal embossing printer, and 3D printing. The Learning Boards were produced in A3 format, using 180 g/m² paper. In addition to the printed materials, alternative materials such as wool, EVA, and others were also used to enhance tactile perception. As a supplementary resource, QR codes containing brief audio explanations of the content were incorporated into a specific quadrant of the learning board, allowing students to locate them independently and play the audio using a cell phone. The Learning Boards were used during classes by two blind students, who reported difficulties in following the theoretical lessons. The greater engagement and participation of these students in the activities constituted one of the criteria for validating the proposed pedagogical resource. The students also highlighted that the audio content contributed significantly to learning, since text-to-speech applications often fail to adequately decode chemical equations. The resource was also evaluated by the course professor, a professor specializing in Braille, and the institution's Braille specialist. It is concluded that the proposed pedagogical resource presents pedagogical coherence and relevance, configuring itself as an assistive technology resource that enables the active participation of students in the construction of chemical knowledge.

Agradecimentos/Acknowledgments

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Teaching Organic Functions through Game-Based Learning (GBL): an Active and Interactive Approach.

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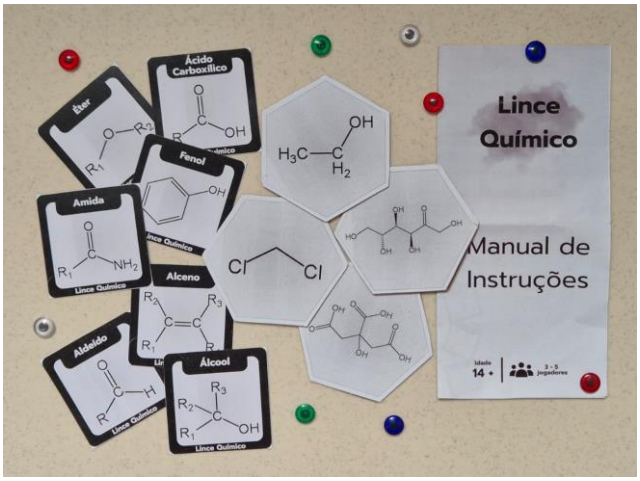
Palavras Chave:*Organic Functions,Teaching Methodologies,Game-Based Learning,Chemistry Education*

Highlights

Game-Based Learning, grounded in Ausubel's theory, is applied to teaching organic functional groups through the Lince Químico game, promoting meaningful learning.

Resumo/Abstract

The teaching of organic functions is often identified as a challenge in the Chemistry learning process, due to the abstract nature of molecular structures and the difficulties students face in establishing conceptual relationships between different functional groups. In light of David Ausubel's Meaningful Learning Theory (2000), teaching is more effective when new knowledge is anchored in previously consolidated cognitive structures relevant to the learner. Game-Based Learning (GBL) embodies this principle by providing contextualized, playful experiences that activate prior cognitive schemas, thus promoting the progressive assimilation of abstract chemical concepts (Prensky, 2001). In this context, the didactic game*Lince Químico*is presented as a strategy for cognitive and functional interactivity (Salen & Zimmerman, 2012), designed to promote meaningful learning of organic functions. The resource is intended for students aged 14 and over, with planned application from the second year of high school onwards. The game consists of cards depicting various organic molecules, through which students identify the functional groups present and establish relationships between chemical structures and their respective functional classifications. The teacher acts as a mediator, responsible for leading conceptual discussions, systematizing the content covered, and relating organic functions to their properties and everyday applications. Although the proposal has not yet been implemented,*Lince Químico*demonstrates pedagogical potential to foster conceptual understanding through a dynamic and interactive approach to teaching Organic Chemistry (Mortimer, 2000).



Representation of the Lince Químico game used in a Game-Based Learning (GBL) teaching proposal

Agradecimentos/Acknowledgments

CAPES, UFES,CNPq, GOVERNO DO ESTADO DO ESPÍRITO SANTO

Teaching Qualitative Chemical Analysis via Didactic Sequence: Detection of Milk Adulterants Through Active Methodologies

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[1]Fundação Indaiatubana de Educação e Cultura

Palavras Chave:*Ensino por Problemas,Análise Qualitativa,Metodologias Ativas,Contextualização*

Highlights

Didactic sequence in Qualitative Chemistry using Problem-Based Learning
Detection of NaOH and Formaldehyde in milk
Student engagement through the development of low-cost colorimetric tests

Resumo/Abstract

Chemistry education in technical and technological courses requires strategies that integrate theory and practice through professional contextualization. In this context, the use of didactic sequences based on active methodologies allows students to take a leading role in solving real-world societal problems. In this scenario, this study was based on a Didactic Sequence (DS) applied to the Qualitative Chemical Analysis discipline, using the theme "Milk Fraud" through the lens of Problem-Based Learning (PBL). The proposal aimed to engage students in solving real food security issues by developing and applying a DS for adulterant detection, training them in performing colorimetric tests and adapting protocols in resource-limited settings. The DS was structured in four stages: 1) Theorization on food fraud and the role of analytical chemistry in this scenario; 2) Study of acid-base equilibria and colorimetric reactions; 3) Laboratory practice with milk samples intentionally contaminated with NaOH (concentrations from 0.1% to 1.0% w/v) and Formaldehyde (0.01% to 0.05% v/v), mimicking real adulterations, using filter papers impregnated with bromothymol blue, phenolphthalein, methyl orange, and Schiff's reagent (synthesized via commercial fuchsine solution); 4) Closing with the elaboration of reports and discussions. During the classes, students participated actively, demonstrating high engagement in transposing pH concepts and organic reactivity into the visual detection of contaminants. The Schiff test revealed formaldehyde through a color change to violet, while the triad of indicators confirmed alkalinization by NaOH (blue/pink/yellow). Finally, the methodology favored autonomy, and the integration between DS and PBL in qualitative analysis proved effective for teaching, consolidating technical learning and stimulating students' critical thinking.

Agradecimentos/Acknowledgments

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Thematic Approach to the Three Pedagogical Moments in Chemistry/Science Teaching: using marolo as a problem-solving theme

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Palavras Chave:*Three Pedagogical Moments,Chemistry/Science Teaching,Didactic Sequence,Marolo.*

Highlights

The didactic sequence, conducted using the Three Pedagogical Moments and employing*marolo*as a problem-solving theme, facilitated the contextualization of the chemistry content being addressed.

Resumo/Abstract

This paper reports on the use of the Three Pedagogical Moments dynamic (Problematization, Organization, and Application of Knowledge) proposed by Delizoicov, Angotti, and Pernambuco (2011) for the planning and implementation of a didactic sequence (DS) with first-year high school students in a private school in a city in southern Minas Gerais, using*marolo*(*Annona crassiflora*), a characteristic regional fruit, as the problematizing theme. As part of the DS activities, an experiment was conducted to investigate the presence of lipids and carbohydrates in the*marolo*, as well as its organoleptic properties. In addition, students were asked to work in groups to create a reinterpretation of a film trailer of their choice, which should involve the theme of the fruit, the chemical and biological concepts related to it, and the socioeconomic importance of the fruit to the city. Regarding the experimental activity, the students were questioned about the properties of*marolo*, and all were able to identify its distinctive flavor and intense aroma, texture, and the presence of lipids and carbohydrates through paper tests and glycosylates. This result aligns with Passos et al. (2022), who indicate that experimental activities contribute to visualizing a situation, causing the student to observe and analyze the results, making them more reflective. The activity of reinterpreting the trailer was successfully produced by the groups, emphasizing the nutritional aspects (micro and macronutrients of the*marolo*), highlighting the biome to which it is native – the Cerrado – its application in typical foods, as well as its presence in cultural attractions that occur in regional festivals, which positively impact the city's economy. The use of a regional theme – in this case,*marolo*– can contribute to student learning by bringing their reality closer to the chemical content, favoring contextualization, making them participative and reflective.

Agradecimentos/Acknowledgments

CAPES; LAPEQUIM – Laboratório de Pesquisa em Educação Química – UNIFAL-MG.

The role of modelling activities in teachers' initial formation and acquisition of knowledge in organic chemistry

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Palavras Chave:*Modeling,Models,Organic Chemistry,Teachers' Formation*

Highlights

Modeling connects chemical knowledge levels. Pre-service teachers got involved in modeling activities for Organic Chemistry. Activities enhanced learning.

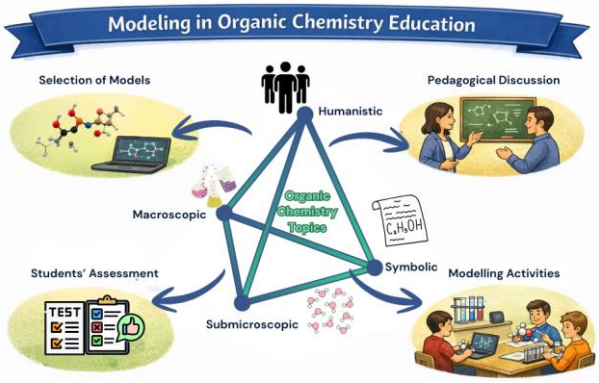
Resumo/Abstract

Introduction: According to Johnstone (1993), later expanded by Sjöström and Talanquer (2014), chemical knowledge can be understood through four complementary levels, which describe chemical phenomena from different perspectives: macroscopic, submicroscopic, symbolic, and humanistic approaches. Students in both basic and higher education are expected to move between these levels, a process in which models play a central role. Models are a fundamental component of chemical knowledge and education and may take several forms, including equations, diagrams, verbal descriptions, virtual simulations, and various forms of physical representation. The construction of models by learners, known as modeling, involves iterative processes similar to scientific inquiry. Despite its educational relevance, studies addressing modelling activities in the initial education of chemistry teachers remain scarce, particularly in Organic Chemistry, a field often taught in an abstract and decontextualized manner in basic education, which could be addressed by modeling activities.

Objective: This study presents and analyzes six modelling activities developed with undergraduate pre-service chemistry teachers.

Methodology: The activities addressed six introductory topics - molecular geometry, organic functions and properties, planar isomerism, acidity and basicity, conformational analysis, and stereochemistry, using models selected from the literature or adapted for the study. Each activity involved a brief pedagogical discussion followed by a modelling task. Data were collected through qualitative records of student responses and pre- and post-tests with open-ended questions.

Results and discussion: The participants positively evaluated the models and modeling's didactic potential, and were able to propose similar activities for future classroom use. The analysis of the tests indicated a mean relative learning gain of approximately 64%.



Integrating different perspectives of chemical knowledge through modeling.

Agradecimentos/Acknowledgments

The authors would like to thank CAPES for providing D.T.'s graduate scholarship and the colleagues from GPEQ for their help.

TOUCH AND ASSOCIATE: LEARNING CHEMISTRY THROUGH TOUCH AND MEMORY

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Palavras Chave:*Inclusion, Braille, Chemical properties, Card game.*

Highlights

Touch and Associate is an accessible game that teaches Chemistry to visually impaired students using Braille cards, promoting tactile learning, chemical property association, and scientific inclusion.

Resumo/Abstract

*Touch and Associate*is an accessible instructional tool designed for teaching Chemistry to students with visual impairments, focusing on the association between chemical elements and physicochemical properties, such as fragility, density, reactivity, and malleability, through Braille cards and tactile resources. Its objective is to promote meaningful learning and inclusion by enabling the development of sensory and cognitive perception of chemical concepts through multisensory approaches. The game consists of a tactile board labeled in Braille from 1 to 6 and from A to F, which supports the localization and organization of the cards. Each card also presents, in Braille, the name and symbol of a chemical element or a corresponding physicochemical property, as illustrated in Figure 1. Inspired by traditional memory games, players are required to form correct pairs between elements and properties during gameplay, using touch and tactile memory as primary cognitive strategies. The rules allow participation by 2 to 6 players, who, in their turns, select board positions, verbalize their choices, and share information with other participants, fostering collaborative learning. Correct matches generate points, and the winner is the player who forms the greatest number of pairs by the end of the game. The methodology emphasizes participatory design in inclusive classrooms, enabling the observation of interactions, cognitive strategies, and learning processes in real time. The game functions as a pedagogical resource that helps overcome barriers in Chemistry education by promoting accessibility, engagement, and equal educational opportunities.



Game card template.

Agradecimentos/Acknowledgments

IFCE – Campus Aracati

PIBID – Sub-projeto Química – IFCE – campus Aracati

LEMA – Laboratório de Ensino Maker do Aracati

CAPES

Uma análise de séries históricas da associação do desempenho na Olimpíada de Químicade São Paulo com fatores associados à desigualdades

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Palavras Chave:*Olimpíada científica, desigualdades, Acesso ao ensino superior,Olimpíada científica, desigualdades, Acesso ao ensino superior,Olimpiada Científica,Desigualdades,Acesso ao ensino superior*

Highlights

Student performance in the São Paulo Chemistry Olympiad is associated with school infrastructure, socioeconomic status, and participation history, possibly reflecting educational inequalities.

Resumo/Abstract

Desde 1997, a Olimpíada de Química de São Paulo (OQSP) tem como primeira etapa a produção de redações abordando temas relacionados à química. Apesar da inscrição ser livre para alunos a partir do 9º ano de qualquer escola do estado, por anos o evento ficou restrito a poucos estudantes, majoritariamente do ensino privado. Entre 2015 e 2019, o número médio de redações foi de 375, sendo apenas 26% provenientes de escolas públicas. Após a pandemia da COVID-19, esses valores cresceram consideravelmente, atingindo em 2025 1792 redações, sendo 63% de escolas públicas. Uma possível influência para esse crescimento pode ter sido a implementação recente das “vagas olímpicas” como via de acesso a universidades. Considerando que outras vias de acesso, como o ENEM, são afetadas por desigualdades[1], buscamos identificar se o mesmo ocorre na OQSP. Para isso, realizamos uma análise estatística comparando o desempenho de estudantes na olimpíada entre 2021 e 2025 com fatores relativos às suas escolas de origem, provenientes do Censo Escolar do INEP, do ENEM, do IDEB e do Indicador de Nível Socioeconômico do INEP (INSE). Consideramos distribuições significativas (t de Student, ANOVA e χ^2 com $p < 0,05$). Identificamos então os fatores relevantes ao longo da série histórica. Em todo o período, o melhor desempenho mostrou-se associado a escolas privadas, com bibliotecas, laboratórios de ciências, profissionais de saúde contratados e com mais participações na OQSP na última década. Em quatro das edições, a presença de ateliês e salas de música também se mostrou relevante. Essas associações se repetem entre escolas públicas. Concluímos que o desempenho na OQSP parece estar associado a escolas com melhor infraestrutura, níveis socioeconômicos mais elevados e tradição de participação na olimpíada, sugerindo que a competição constitui mais um contexto em que se manifestam as desigualdades educacionais.

1. SENKEVICS, A. S. et al. Cadernos de Pesquisa, v. 52, p. e09528–e09528, 2022.

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Uma sequência didática envolvendo radioatividade: concepções críticas do alunado sobre o poema a rosa de Hiroshima

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Palavras Chave:*ensino médio,radioatividade,sequência didática,CTSA,a rosa de Hiroshima*

Highlights

Science-Technology-Society-Environment conception into a didactic sequence involving a discussion about the poem The rose of Hiroshima, showed a potential to increment the learning about radioactivity

Resumo/Abstract

O ano de 2026 marca quatro décadas do desastre nuclear de Chernobyl. Com o conflito Rússia–Ucrânia e aspectos geopolíticos atuais é imperativo evocar o tema radioatividade, sob a concepção ciência-tecnologia-sociedade-ambiente (CTSA). Assim, uma sequência didática (SD) do tema foi aplicada a estudantes de segunda série do ensino médio, com abordagens expositivo-dialógicas, seminários e um debate sobre o poema a rosa de Hiroshima. O trabalho relacionou duas questões debatidas pelos aprendizes e uma ilustração, presentes em cada entrega por grupo (32 grupos/81 discentes), que trouxeram relações com a bomba de Hiroshima, a radioatividade e uma produção visual. Ilustrações de rosa estiveram em 30 das entregas. Alusão a guerra/dano material (em 21), dano a saúde ou morte (em 20), simbologia nuclear ou de risco biológico (em 12) também surgiram.
O relato iniciou a SD, possibilitando diagnosticar o referencial histórico do alunado, aspectos atitudinais e habilidades de leitura-interpretação-escrita. O debate inicial deles tratou da menção de “chuva radioativa” – típica de ficções na guerra fria –; ilustrações em quadrinhos, sequenciados por trechos do poema como “pensem nas crianças || mudas telepáticas”, observando a destruição; a rosa como símbolo de sobrevivência diante da destruição; e a intertextualidade, com menção a filme sobre aspectos pós-guerra.
A relação arte e ciência converge, pertencendo a processos/produtos do pensamento humano da mesma busca imaginativa, apesar de se expressarem com linguagens diferentes. O poema tratado surgiu por inspirações do mau uso da radioatividade, propondo críticas ao processo científico, e alia o papel estético-artístico ao ensino de ciências, principalmente nos aspectos CTSA do porquê de se fazer ciência e de tudo que interfere nessa prática. Com a SD foram explorados aspectos de sociabilização, coletividade, argumentação e criatividade, relevantes para a condução dos objetivos educacionais e fortalecimento do processo de ensino.

Uma Sequência didática sobre o ensino de biomoléculas através da merenda escolar

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Palavras Chave:*Biomoléculas,Funções Orgânicas Nitrogenadas,Ensino de química.,Biololeculas,Ensino de Química,Funções nitrogenadas e oxigenadas.*

Highlights

The study aims to connect concepts of carbohydrates, proteins, and lipids to the reality of students. The guiding question of this study is: "Do you really know what you're eating for lunch at schoo?"

Resumo/Abstract

O ensino de Química Orgânica desempenha papel fundamental na construção do conhecimento científico, tanto no âmbito escolar quanto em contextos externos à sala de aula. Contudo, observa-se que, frequentemente, esse conteúdo é ministrado de forma descontextualizada, com predominância de abordagens estritamente teóricas. Tal prática compromete a compreensão de conceitos essenciais à formação dos estudantes, uma vez que estes, em grande parte, não conseguem estabelecer relações entre os conteúdos trabalhados em sala e situações concretas de seu cotidiano. Essa desconexão contribui para a ausência de motivação no processo de aprendizagem, reforçando a necessidade de metodologias que promovam maior integração entre teoria e prática. Assim, com o intuito de contribuir para a melhoria do ensino de química Orgânica esse trabalho investiga o uso da merenda escolar como estratégia para o ensino do conteúdo de biomoléculas (carboidratos, proteínas e lipídios) para elaboração de uma Sequência didática (SD). A proposta foi estruturada segundo os Três Momentos Pedagógicos (Problematização Inicial, Organização do Conhecimento e Aplicação de Conhecimento) e aplicada a uma turma de 28 estudantes de uma escola pública de Natal–RN. Os instrumentos de coleta de dados quantitativos foram dois questionários. Observou-se, inicialmente, dificuldades na identificação de funções químicas como: I) a não distinção entre aldeídos e cetonas, II) na relação entre alimentos e biomoléculas e III) na classificação do álcool secundário. Ao final da aplicação da SD observou-se uma melhora no número de acerto de questões, esse incremento não pode ser interpretado como resultado consolidado do processo de ensino aprendizagem, mas sim de pelo menos uma evolução na identificação das funções estudadas. Identificou-se ainda que as questões mobilizam competências e habilidades previstas no ENEM, especialmente as competências de área C5, C6 e C7, associadas às habilidades H17, H18, H19, H21, H24 e H25.

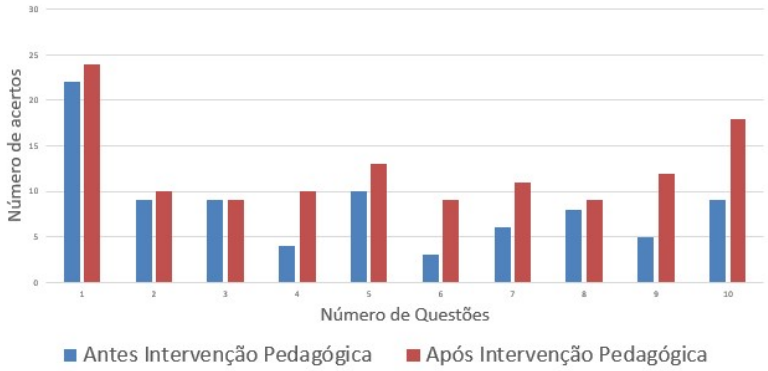


Figura 1 - Quantidade de acerto das 10 questões de multipla escolha

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What do studies on Artificial Intelligence in Chemistry teaching reveal? An analysis of scientific publications from 2022 to 2025

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Palavras Chave:*Chemistry Teaching,Artificial Intelligence,Chatbots,Systematic literature review*

Highlights

Systematic review analyzed AI research in Chemistry Teaching published between 2022 and 2025. Studies stress AI potential, limits, with only 11 articles address the topic, revealing limited production

Resumo/Abstract

The increased use of Artificial Intelligence (AI) in education, especially since the popularization of generative models, has sparked debates about its impacts on knowledge construction. In Chemistry Teaching (CT), research has sought to describe the use of Generative AI in teaching and learning processes. In this context, this research aimed to analyze the core of articles published between 2022 and 2025 that involve AI and CT, seeking to identify trends, theoretical and methodological approaches, and the contributions of these productions. To this end, a qualitative research design was adopted, and a systematic literature review (SLR) was conducted in five stages: 1) Definition of the research question (What has been the core of articles in Chemistry teaching involving AI?); 2) Selection of the database (Google Scholar), inclusion criteria (articles in Portuguese), and exclusion criteria (theses, dissertations, monographs, and conference proceedings), and keywords (AI and CT); 3) Selection of studies; 4) Analysis and synthesis of the studies included in the SLR; 5) Writing and publication of the findings. The results show that, although Google Scholar presents a substantial volume of publications on AI and education, only 11 articles met the specific criteria related to CT. The analysis of these studies revealed that the core of the investigations focuses, mainly, on evaluating the potential of chatbots for: defining chemical concepts, solving exercises, developing lesson plans, supporting teacher planning, and mediation of learning. It was observed that the articles highlight both the potential of AI and its conceptual limitations, especially in content that requires mathematical and chemical rigor. The importance of teacher mediation and the critical use of AI is also emphasized across the articles. It is concluded that scientific production in Portuguese on AI in Chemistry Teaching, although growing, is still incipient and predominantly exploratory.

Agradecimentos/Acknowledgments

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"Who am I in the periodic table?": a hybrid and synchronized game for inclusive teaching of the periodic table.

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Palavras Chave:*Periodic Table, Digital Technologies, Inclusion,Periodic Table,Digital Technologies,Inclusion*

Highlights

The game integrates physical cards and a real-time digital interface, uses Firebase, provides Braille accessibility features, and promotes active, inquiry-based learning of periodic properties.

Resumo/Abstract

This work presents the development of a hybrid pedagogical tool for teaching the Periodic Table, entitled “Who Am I in the Periodic Table?”, whose source code is publicly available on GitHub, ensuring transparency and reproducibility. The proposal aims to replace memorization-based practices with an inquiry-based approach, employing web technologies (HTML5, Tailwind CSS, and JavaScript) integrated with the Firebase Realtime Database to enable real-time synchronization across devices. The game dynamics are based on logical elimination: initially, the system randomly selects 24 elements displayed in the virtual interface, as illustrated in Figure 1. Based on this selection, student groups organize the physical game by separating only the cards corresponding to the selected elements. The game progresses through rounds of questions addressing chemical and periodic properties (e.g., “Does your element belong to the alkali metals?”). After each response, students perform a coordinated action, simultaneously eliminating candidates on both the physical board and the digital interface. This action updates the cloud database and synchronizes progress among participants with no perceptible latency. The analysis of the system architecture and its experimental application at IFCE Campus Aracati indicate a high potential for student engagement, promoting the recognition of chemical symbols, periodic properties, and classification patterns. The proposal is further distinguished by its commitment to inclusion, implemented through Braille-adapted physical cards and the use of ARIA attributes in the digital interface, which allow autonomous interaction by visually impaired students via screen readers. It is concluded that the tool constitutes an effective didactic resource, integrating chemical concepts with Information and Communication Digital Technologies in a meaningful and accessible manner..

QR Code for accessing the virtual game.

Agradecimentos/Acknowledgments

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ELE - Eletroquímica e Eletroanalítica

Activated carbon electrodes derived from purple corn cob (Zea mays L.) for coin-cell supercapacitors

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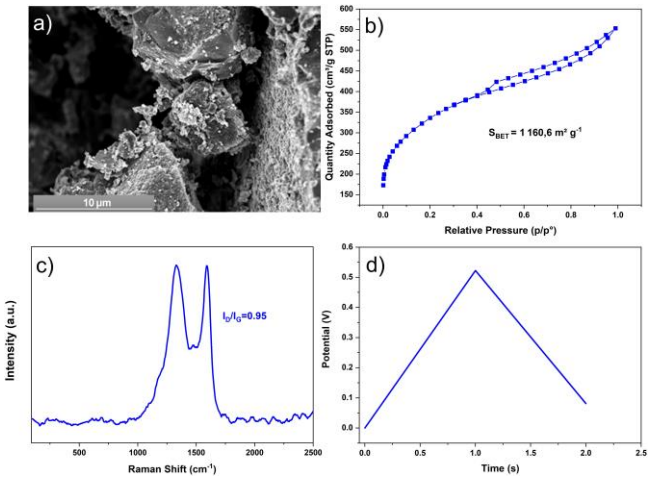
Palavras Chave:*activated carbon,purple corn cob,supercapacitors,electrode,coin cell*

Highlights

Purple corn cob activated carbon (H_3PO_4, 700 °C) reached S_BET = 1160.6 m^2 g^{-1}, delivering 96 F g^{-1}(3-electrode) and 30 F g^{-1}in coin-cell supercapacitors.

Resumo/Abstract

Sustainable and low-cost electrode materials are essential for advancing supercapacitors (SCs) toward practical and scalable energy storage applications. Biomass-derived activated carbons are particularly attractive due to their tunable porosity, high surface area, and the possibility of obtaining high-performance electrodes from renewable resources. Herein, we report the preparation and study of carbonaceous materials for coin-cell supercapacitor assembly using purple corn cob (Zea mays L.) as the raw material. The biomass was chemically activated with H_3PO_4 at concentrations of 1, 4, and 8 mol L^{-1} and pyrolyzed at 700, 800, and 900 °C under an N_2 atmosphere. The resulting carbons, labeled CAMM–H_3PO_4, were physicochemically characterized using Fourier-transform infrared (FT-IR) spectroscopy, Raman spectroscopy, scanning electron microscopy (SEM), and N_2 adsorption/desorption analysis. Their electrochemical behavior was evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge–discharge (GCD) tests in a three-electrode Swagelok cell using 5 mol L^{-1} KOH as the electrolyte. The CAMM–H_3PO_4 electrode treated at 4 mol L^{-1} and 700 °C exhibited the best electrochemical performance, showing a well-developed porous structure (Fig. 1a), a high specific surface area (SBET = 1160.6 m^2 g^{-1}; Fig. 1b), and an ID/IG ratio of 0.95 (Fig. 1c). In the three-electrode configuration, this material delivered 96 F g^{-1} at a current density of 0.2 A g^{-1}. In contrast, the coin-cell device exhibited a capacitance of 30 F g^{-1} at a current density of 0.25 A g^{-1}. These results demonstrate that CAMM–H_3PO_4 electrodes exhibit strong potential for application in practical energy storage systems.



(a) SEM of CAMM–H_3PO_4; (b) N_2 isotherm; (c) Raman; (d) GCD in 5 mol L^{-1} KOH (3-electrode Swagelok).

Agradecimentos/Acknowledgments

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Adding value to sugarcane vinasse through microbial fuel cell for energy generation and ammonium recovery

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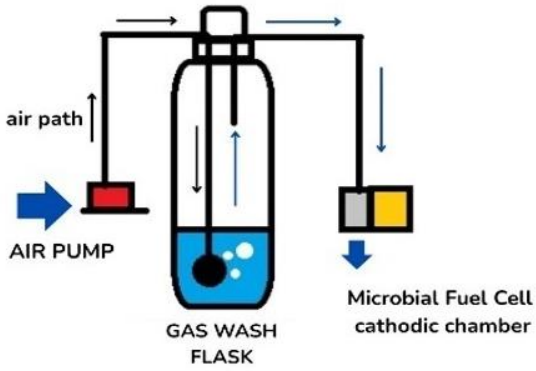
Palavras Chave:*Microbial fuel cell,Sugarcane vinasse,Ammonium,Energy generation*

Highlights

An innovative microbial fuel cell treats vinasse, recovers ammonium, and generates electricity with formation of a conductive and stable biofilm.

Resumo/Abstract

Brazil is one of the world's largest sugarcane producers of bioethanol. This activity generates vinasse, a liquid residue which is applied as land fertilizer. But its directly use to the soil causes land imbalance and salinization. Thus, technologies to recover nutrients could give a rational destination to this wastewater and help an important agro-industrial sector. Herein, we developed a microbial fuel cell (MFC) to treat vinasse, recover total ammonia nitrogen with simultaneous energy generation. The experiments were carried out in a dual chamber acrylic cell, with anode and cathode compartments separated by a Nafion® membrane hot-pressed with carbon cloth with 40% Pt (cathode-15 cm^2). The anode was a carbon brush connected to a titanium rod. Initially, MFC was inoculated with a sludge obtained from an anaerobic digestor of vinasse from a sugarcane plant located in Pradópolis-SP, and connected to an external resistance (Rext) of 1 kΩ. The MFC was initially operated with a substrate containing ammonium acetate at 2 $g.L^{-1}$ (A-Ac) in Lovley-Phillips medium, yielding an output voltage of 800 mV and a maximum power density of 250 $mW.m^{-2}$. Electrochemical impedance spectra (EIS) in the presence and absence of the biofilm showed a reduction in charge transfer resistance (Rct) from 22.8 kΩ to 2.5 Ω, showing formation of a conductive biofilm. To investigate the dynamics of ammonium transport, the system was operated under different Rext values. The maximum ammonium transport rate from the anode to the cathode reached 28% and 19%, respectively, at open-circuit potential and Rext = 330 Ω. To mimetites real wastewater treatment, acetate has been replaced by vinasse sugarcane (6% v/v); the vinasse-MFC showed an output voltage of 658 mV and a maximum power density of 80 $mW.m^{-2}$. To date, the transition to vinasse has shown promising results, so further electrochemical analyses and the efficiency of ammonium recovery from vinasse are underway.



MFC setup.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge the financial support provided by the São Paulo Research Foundation - FAPESP (Grant numbers: 2024/12971-5, 2023/07992-0, 2021/12866-9, and 2024/00725-0).

A Statistical Framework for Multi-Response Analyses: Comparison of Activated 3D-Printed Carbon Black/Polylactic Acid Electrodes

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Palavras Chave:*Additive Manufacturing,3D-Printed Electrodes,Surface Activation,Statistical Framework,Multi-Response Analysis*

Highlights

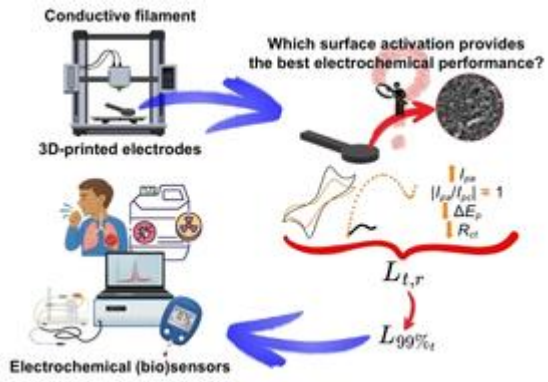
Risk-adjusted metric unifies normalized variables for performance and reproducibility;

NaOH-ECNaOH and NaOH were the best protocols;

The framework is generalizable to any multi-response problem.

Resumo/Abstract

Additive manufacturing using conductive filaments enables the rapid fabrication of electrochemical (bio)sensors. However, the insulating polymer matrix frequently requires surface activation to expose conductive fillers, a step that is often statistically overlooked. In this context, a multi-response framework was developed in this work to compare chemical (DMF, H2SO4, and NaOH), electrochemical (ECPBS and ECN_aOH), and combined activation protocols (chemical followed by electrochemical treatment) applied to 3D-printed carbon black/polylactic acid (CB/PLA) electrodes, using the $[Fe(CN)6]^{3-/4-}$ redox probe. Levene's test across scan rates revealed heterogeneous variances among electrochemical responses, motivating normalization and weighting of key variables (anodic peak current, current ratio, peak-to-peak separation, and charge transfer resistance) into a unified performance index (L), which was further converted into a risk-adjusted score ($L_{99}\%=L-k\cdot\sigma L$, where k= 2.35 for 99% confidence) to penalize variability across replicates. The variances of L and $L_{99}\%$ were homogeneous across scan rates but heterogeneous among treatments, indicating that scan-rate modulation does not introduce differential variability, whereas surface treatment is the major factor governing average performance. Thus, a global score integrating data from all scan rates was adopted to assess overall performance, identifying protocols that balance performance and reproducibility. The NaOH-ECN_aOH treatment delivered the highest score ($L_{99}\%$= 0.90 versus 0.14 for the untreated samples), while the simpler single-step NaOH showed a comparable value ($L_{99}\%$= 0.86), offering a technically attractive alternative. Sensitivity tests with weights (0.2–0.4) preserved rankings, confirming the framework stability and robustness. This approach is generalizable to other multi-response optimization contexts, including conductive materials, (bio)sensing interfaces, surface engineering, and filament aging studies.



Workflow for fabrication, activation, and electrochemical evaluation of 3D-printed electrodes.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from CAPES, CNPq, and FAPERJ. They also thank PEQ/COPPE/UFRJ, LABEFIT, and NANO&UFRRJ for institutional support and research facilities.

A three-component carbon nanotubes/MoS_2/Prussian blue nanocomposite cathode for aqueous potassium-ion batteries

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Palavras Chave:*Nanocomposites, Molybdenum Disulfide, Prussian blue, carbon nanotubes, aqueous batteries.,Nanocomposites,Molybdenum Disulfide,Prussian blue,carbon nanotubes,aqueous batteries*

Highlights

Thin films of a nanocomposite composed of carbon nanotubes (CNTs), molybdenum disulfide (MoS_2) and Prussian blue for application as electrodes in aqueous potassium-ion batteries.

Resumo/Abstract

Alternatives to conventional lithium-ion batteries that are more efficient, safer, sustainable and cost-effective have attracted increasing attention in recent decades due to the growing global energy demand. In this context, aqueous potassium-ion batteries emerge as a promising option, as they potentially combine all these features. This work reports the synthesis of a novel nanocomposite composed of carbon nanotubes (CNTs), molybdenum disulfide (MoS_2) and Prussian blue (PB), aiming at its application as a cathode material for aqueous potassium-ion batteries. Thin films of CNTs and MoS_2 were initially prepared via the liquid–liquid interfacial route (LLIR) and subsequently used as precursors for the electrochemical synthesis of PB, leading to the formation of the three-component composite. The electrodeposition process was investigated under different pH conditions and potential windows. The resulting materials were characterized by UV–Vis spectroscopy, Raman spectroscopy, scanning electron microscopy (SEM), and electrochemical techniques. The results confirmed the successful formation of the nanocomposite, with intimate contact among the three components and preferential PB growth on MoS_2 flakes, in contrast to control films without MoS_2. Notably, the presence of MoS_2 enabled composite formation under pH and potential conditions unfavorable for PB electrodeposition in its absence. Electrochemical stability tests conducted by continuous cyclic voltammetry in KCl 0.1 mol L^{-1} revealed enhanced stability for the tricomponent sample obtained at pH 2, with an 11% improvement compared to the control. Galvanostatic charge–discharge measurements demonstrated typical battery behavior, delivering a specific capacity of 160 mAh g^{-1} in 0.5 mol L^{-1} KCl within a potential window of 0.0–0.6 V, corresponding to a 28% increase relative to the control film.
Schmidt, A. et al, Electrochimica Acta, 387, 138500, 2021.
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Agradecimentos/Acknowledgments

CAPES, CNPq, INCT-Nanovida and INCT-Nanocarbono.

Avaliação eletroquímica de eletrodos de feltro de carbono modificados visando aplicações em baterias de fluxo redox

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Palavras Chave:*Feltros de Carbono, "RFBs", Eletrodos Modificados, Eletrólitos de Vanádio.,Feltros de Carbono, "RFBs", Eletrodos Modificados, Eletrólitos de Vanádio*

Highlights

Thermal Electrode activation

Electrode Modification with Niobium and Tungsten oxide,

Cyclic Voltammetry evaluation.

Resumo/Abstract

Frente ao impacto ambiental associado às baterias de íon-lítio, torna-se essencial o desenvolvimento de alternativas mais sustentáveis, como as baterias de fluxo redox (RFBs). Embora promissoras para aplicações estacionárias de armazenamento de energia, essas tecnologias ainda demandam estratégias de otimização para melhorar seu desempenho eletroquímico. Nesse contexto, este trabalho apresenta um estudo comparativo de diferentes modificações em eletrodos de feltro de carbono (FC), com o objetivo de aumentar a densidade de corrente do sistema. Foram avaliadas duas estratégias de ativação térmica: tratamento químico em H_2SO_4 seguido de aquecimento a 400 °C (12 h, em ar) e tratamento térmico direto a 530 °C (2 h, em atmosfera de N_2). Adicionalmente, os eletrodos foram modificados com óxidos metálicos contendo Nb/W por meio da imersão dos FC em solução de $NH_4[NbO(C_2O_4)_2(H_2O)]\cdot H_2O$ e $(NH_4)_2WS_4$ (10:1, 1 h), seguida de calcinação a 530 °C (2 h, N_2). As análises voltamétricas foram conduzidas em eletrólito de vanádio (14 mmol L^{-1}), em um sistema de três eletrodos: FC (trabalho), tarugo de carbono (contra-eletrodo) e Ag/AgCl (KCl sat.) como eletrodo de referência. Os voltamogramas cíclicos evidenciaram dois processos eletroquímicos associados aos pares redox V^{4+}/V^{5+} e V^{3+}/V^{2+}. Observou-se que os eletrodos tratados a 400 °C e o eletrodo controle apresentaram maiores correntes para o par V^{4+}/V^{5+}, enquanto o eletrodo modificado e o tratado a 530 °C exibiram maior resposta para o par V^{3+}/V^{2+}, além de menor separação de picos, indicando maior reversibilidade do sistema. Os resultados demonstram que o protocolo de ativação ou modificação influência de forma distinta o comportamento eletroquímico dos pares redox. Trabalhos futuros visam avaliar a incorporação de outros óxidos metálicos e a integração desses materiais em protótipos de células de fluxo.

LI, Bin, et al. Nano Letters, v. 14, p. 158-165, 2014.

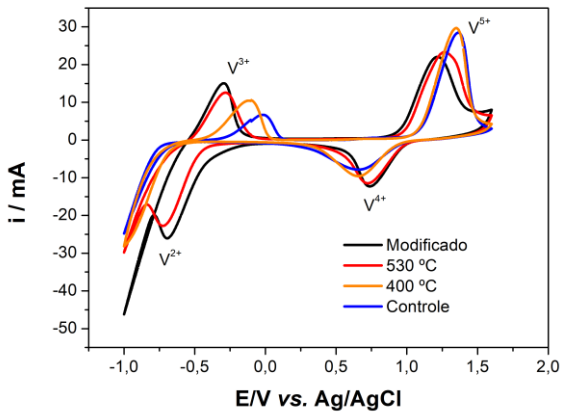


Fig.1: Voltamogramas dos eletrodos de FC após diferentes tratamentos e modificação. v = 10 mV/s

Agradecimentos/Acknowledgments

Agradecemos ao CNPq pelo apoio financeiro e pela concessão de auxílio à pesquisa (Processo nº 446787/2024-8, 314945/2025-3, 192408/2025-9).

Da prospecção à barragem: análise eletroanalítica de metais potencialmente tóxicos em rejeito de mineração de ouro.

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Palavras Chave:*Mineração de ouro,Eletroquímica,Rejeito de mineração,Eletrodo quimicamente modificado,Metais potencialmente tóxicos*

Highlights

A mineração de ouro junto ao beneficiamento, gera grande receita para o Brasil. Porém, há grande produção de rejeito com metais tóxicos, a eletroquímica pode ser usada na determinação dessas espécies.

Resumo/Abstract

O período entre 1610 e 1850 é considerado o momento-chave para a mineração de ouro no Brasil, uma vez que a extração mineral ganhou dimensões nunca vistas e notoriedade na economia nacional. Dado o impacto, em 2020, o país se consolidou como 8° maior produtor de ouro mundial, com uma produção de cerca de 107 t. Atualmente, o papel da mineração permanece relevante, com destaque para o beneficiamento mineral, que consiste em processos físicos e químicos que agregam valor ao minério. Nesse contexto, a cianetação é o método mais utilizado, dado os altos resultados de rendimento e de pureza. Entretanto, esse processo gera uma grande quantidade de rejeitos, tradicionalmente alocado em barragens, o que representa um risco potencial de contaminação ao meio ambiente e à saúde da população. Devido a formação geológica do minério de ouro, esse está usualmente associado a minerais sulfetados que contêm em sua estrutura, ferro, cobre, chumbo e zinco. A determinação da concentração dessas espécies é fundamental para a sua destinação final adequada. Frequentemente, são quantificadas por espectrometria de absorção atômica e de emissão óptica com plasma indutivamente acoplado (ICP-OES); contudo, essas técnicas requerem equipamentos específicos e mão de obra especializada. Com isso, as técnicas eletroanalíticas surgem como uma alternativa, conferindo alta sensibilidade e menor custo. Assim, propôs-se a avaliação de cobre, cádmio, chumbo e zinco em amostras de rejeito usando voltametria linear e de pulso diferencial. A fim de aumentar a sensibilidade do método, utilizou-se um eletrodo de carbono vítreo com um filme de mercúrio. Para a quantificação, realizaram-se curvas analíticas, obtendo-se coeficientes de correlação superiores a 0,9. Para analisar o rejeito, realizaram-se extrações sucessivas, testando-se três extratores, a fim de comparar os resultados obtidos com os determinados por ICP-OES, de modo a acompanhar a liberação dos metais em solução via balanço metalúrgico.

Agradecimentos/Acknowledgments

Agradeço ao Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) pelo fomento do projeto por meio da bolsa PIBIC, ao laboratório LDBC/ LTE pela estrutura fornecida e ao CETEM pela disponibilização das amostras

Desenvolvimento de Eletrodos Eficientes de Papel de Grafeno Modificados com Azul da Prússia para Detecção de H_2O_2

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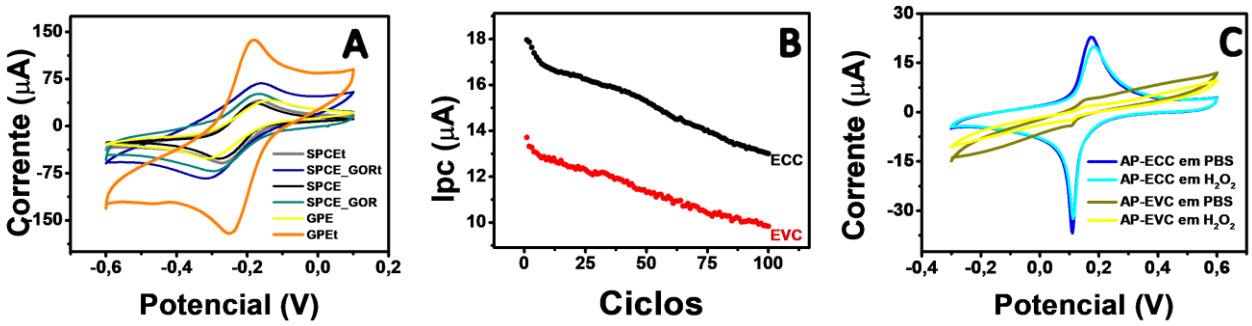
Palavras Chave:*Grafeno; Azul da Prússia; Detecção de Peróxido; Sensor Eletroquímico; Eletrodo de Grafeno.*

Highlights

O eletrodo de papel de grafeno tratado apresentou melhor desempenho eletroquímico que eletrodos convencionais, e a síntese de AP por ECC mostrou maior estabilidade em KCl e melhor resposta ao H_2O_2.

Resumo/Abstract

O papel de grafeno (GPE) combina propriedades eletrônicas e estruturais promissoras, mas costuma ser usado apenas como suporte em sensores amperométricos. O pré-tratamento superficial dos eletrodos é uma estratégia eficaz para melhorar sua resposta eletroquímica. Neste trabalho, investigou-se o efeito de um pré-tratamento eletroquímico sobre o papel de grafeno e sua influência na deposição e desempenho de filmes de Azul da Prússia (PB). O pré-tratamento foi realizado em PBS 0,1 mol·L^{-1} aplicando-se +1,8 V vs Ag/AgCl por 60 s, seguido de −1,8 V por 60 s. O mesmo protocolo foi aplicado ao eletrodo impresso de carbono (SPCE) e ao SPCE modificado por dropcasting com óxido de grafeno reduzido[1]. O GPE tratado (GPEt) apresentou melhora nas propriedades eletroquímicas, evidenciada pelo aumento dos picos redox em voltamogramas em solução de $Ru(NH_3)_6Cl_3$ 5 mmol/L e KCl 0,1 mol/L, Figura 1A, e também maior área eletroativa (3413 ± 376,3 cm²), quando comparado ao GPE (846 ± 60,7 cm²) e ao SPCE (1201 ± 74,4 cm²). A deposição de AP sobre GPEt foi realizada por duas rotas: conversão eletroquímica (ECC) de nanopartículas de δ-FeOOH, aplicando-se 1,6 V vs Ag/AgCl por 450 s, seguido de 0,0 V por 300 s, em eletrólito pH 2,0 contendo δ-FeOOH (0,1 mg/mL) e $K_3Fe(CN)_6$ 0,4 mmol/L em K_2SO_4 0,1 mol/L; e por eletrodeposição voltamétrica (EVC)[2],com ciclagem entre −0,2 e 1,2 V vs Ag/AgCl a 0,05 V/s por 20 ciclos, em solução contendo $K_3Fe(CN)_6$ e $FeCl_3$ 2 mmol/L em KCl 0,1 mol/L e HCl 0,01 mol/L. Ambos os filmes apresentaram estabilidade em KCl 0,1 mol/L (pH ≈ 7,0) Figura 1B, com redução da corrente de pico após 100 ciclos de 27,6% (ECC) e 28,3% (EVC). A resposta analítica ao H_2O_2 foi superior para GPEt/AP-ECC, com redução de 4,3 µA do pico catódico na presença de 100 µmol/L do analito, e 0,9 µA para EVC, Figura 1C. Esses resultados indicam que o pré-tratamento eletroquímico do papel de grafeno, aliado à deposição por ECC, produz um eletrodo (GPEt/AP-ECC) promissor para detecção sensível de H_2O_2.



A) VC´s em $Ru(NH_3)_6Cl_3$. B) Ipc em 100 ciclos em KCl das sínteses de AP. C) VC´s em PBS e H2O2.

Agradecimentos/Acknowledgments

Os autores agradecem às agências de fomento FAPEMIG (APQ-00607-22), CNPq e CAPES, bem como à Universidade Federal dos Vales do Jequitinhonha e Mucuri (UFVJM), pelo apoio financeiro e institucional ao desenvolvimento deste trabalho.

Desenvolvimento em laboratório de materiais precursores para placas negativas de baterias chumbo-ácido: Avaliação estrutural e eletroquímica.

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Palavras Chave:*Bateria chumbo-ácido, Materiais precursores, Sulfatos básicos de chumbo, Preparação em laboratório, Voltametria cíclica.*

Highlights

Preparation of lead-acid battery precursor materials.

Controlled curing and hydrothermal treatments at lab scale.

Structural and electrochemical features linked to precursor morphology.

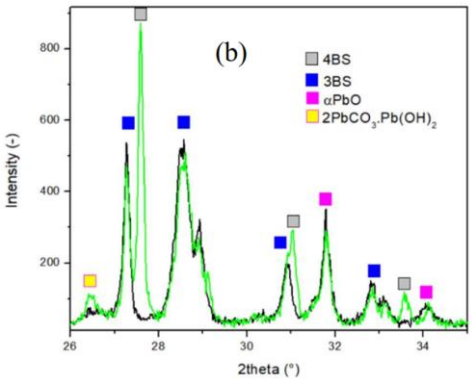
Resumo/Abstract

Este trabalho apresenta o preparo em laboratório de materiais precursores empregados em baterias chumbo-ácido, com ênfase na simplicidade operacional e no controle experimental das etapas envolvidas. Pastas à base de PbO, $3PbO{\cdot}PbSO_4{\cdot}H_2O$ (3BS) e $4PbO{\cdot}PbSO_4$ (4BS) foram obtidas por mistura manual, ajustando parâmetros como temperatura, teor de água, razão H_2SO_4/pó de chumbo e densidade, de modo a reproduzir condições de empaste em escala reduzida. As pastas foram aplicadas manualmente em grades comerciais de Pb/Sb, avaliando-se a viabilidade do processo sem o uso de equipamentos industriais.

As placas empastadas foram submetidas à cura em câmara climática construída em laboratório, com controle de temperatura e umidade relativa. Durante esse processo, ocorreram reações de dissolução e precipitação que promoveram a formação de pescoços entre as partículas da pasta, resultando em uma estrutura contínua e mecanicamente estável, favorecendo a adesão entre o material precursor e a grade metálica, bem como a oxidação parcial do chumbo metálico. A obtenção de material precursor à base de 4BS a partir de 3BS foi realizada por tratamento hidrotérmico a 90 °C, permitindo acompanhar transformações de fase associadas ao crescimento e à reorganização cristalina.

A caracterização dos materiais foi realizada por difração de raios X, análise termogravimétrica e calorimetria exploratória diferencial, evidenciando diferenças estruturais e térmicas entre os materiais preparados. Após a formação eletroquímica, as placas negativas foram avaliadas por voltametria cíclica em solução de H_2SO_4, revelando comportamentos distintos nos processos de formação e redução do filme de $PbSO_4$. Os resultados indicam que variações no preparo dos materiais precursores impactam suas características estruturais e seu desempenho eletroquímico, destacando o potencial dessa abordagem para estudos e desenvolvimento em laboratório.

[1] PAVLOV, D. Lead-Acid Batteries: Science and Technology. Amsterdam: Elsevier, 2011.



Difratogramas das diferentes amostras de material precursor.

Agradecimentos/Acknowledgments

A Tecccer Industria e Comércio de Produtos Cerâmicos. Universidade Federal de Uberlândia.

Development and application of electrochemical sensors obtained by additive manufacturing for pesticide detection

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Palavras Chave:*Additive manufacturing, electrochemical sensors, polypropylene, coconut oil, carbaryl*

Highlights

• Sustainable coconut oil-based conductive filament for 3D printing

• Ready-to-use electrochemical sensor without chemical activation

• Reliable carbaryl detection in environmental water samples

Resumo/Abstract

Additive manufacturing has emerged as a powerful strategy for producing low-cost and customizable electrochemical devices through the development of novel conductive filaments [1,2]. In this work, a sustainable 3D-printed electrochemical sensor was developed using a lab-fabricated filament composed of carbon black (CB), polypropylene (PP), polylactic acid (PLA), and coconut oil for the detection of the insecticide carbaryl in water samples. The filament formulation was based on the CB–PP–PLA conductive system previously reported by Bertolim et al. [3], with coconut oil introduced as a bio-based additive. The lab-made filament was produced via melt mixing, grinding, and extrusion, followed by electrode fabrication using fused deposition modeling (FDM). Morphological, chemical, and electrochemical characterization was performed using scanning electron microscopy, contact angle measurements, FTIR-ATR, Raman spectroscopy, cyclic voltammetry, and electrochemical impedance spectroscopy. The results confirmed homogeneous dispersion and moderate surface hydrophilicity, favorable for electrochemical applications. Mechanical polishing ensured adequate electrochemical performance, eliminating chemical or electrochemical activation. Under optimized parameters, carbaryl detection by square wave voltammetry showed a linear response from 1.0 to 100.0 µmol L^{-1} with a detection limit of 0.25 µmol L^{-1}. The sensor exhibited good repeatability, reproducibility, and satisfactory recoveries (90–105%) in spiked tap and lake water samples. Therefore, the proposed sensor combines competitive analytical performance with reduced fabrication complexity, cost, and environmental impact, highlighting coconut oil-based conductive filaments as sustainable, ready-to-use materials for environmental monitoring.

[1] Stefano, J.S., et al., Anal. Chem., 94, 6417–6429 (2022).

[2] Crapnell, R.D., et al., Materials Today, 71, 73–90 (2023).

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Agradecimentos/Acknowledgments

The authors acknowledge financial support from São Paulo Research Foundation (FAPESP, 2023/06793-4, 2024/16461-1), Funding Authority for Studies and Projects (FINEP, 01.22.0179.00, MARTMA project), and CNPq (401977/2023-4), Brazil.

Development of a 3D-Printed Sensor for Dopamine as a Parkinson's Disease Biomarker

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Palavras Chave:*3D-Printing; Electrochemical sensor; Early detection; Graphite; Castor oil.*

Highlights

3D-printed electrodes lab-made composed of graphite, castor oil and PLA.

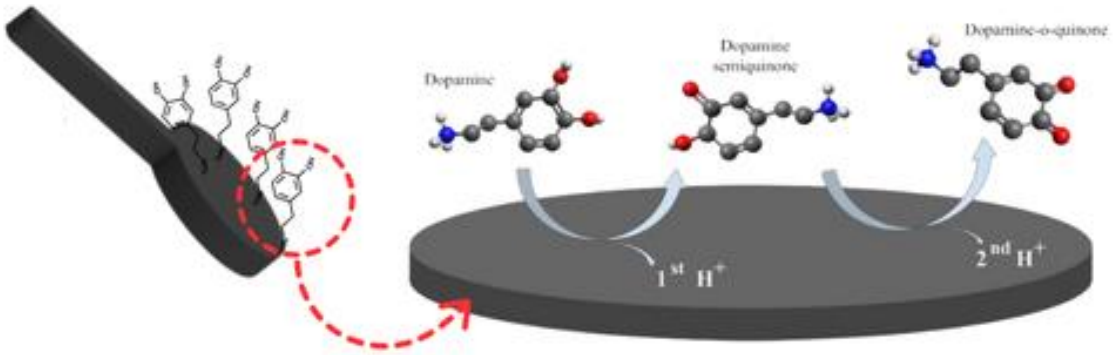
Dopamine was detected using CV and DPV with 0.399 and 0.938 µmol L^{-1} LOD, 1.295 and 1.752 µA µmol L^{-1} cm^{-2} sensitivity.

Resumo/Abstract

Early diagnosis of neurodegenerative disorders like Parkinson's disease is difficult due to subtle early symptoms and complex diagnostic methods[1,2]. Electrochemical sensors offer a promising alternative, as they are low-cost, rapid, and compatible with 3D printing[3,4]. This study develops a 3D-printed, graphite-based sensor for the direct detection of dopamine (DA), a key biomarker in Parkinson's disease. Electrodes were fabricated by dispersing graphite (45% w/w) in castor oil (15% w/w) and polylactic acid, yielding a conductive composite suitable for electrochemical measurements[3,4]. The mass transfer mechanism involved in DA oxidation was assessed by examining the relationship between the logIpa and the logv using cyclic voltammetry (CV), yielding the regression equation $\log I_{pa}$ (µA) = 0.742logv (V s^{-1}) + 2.41 (R^2 = 0.985). The observed slope value (0.742), which exceeds the theoretical value of 0.5 for diffusion-controlled processes, indicates a mixed control mechanism involving both diffusion and adsorption. DA was detected using CV and differential pulse voltammetry (DPV) in 0.1 mol L^{-1} PBS at pH 7. The GR45CO15 electrode achieved limits of detection of 0.399 µmol L^{-1} CV and 0.938 µmol L^{-1} DPV, with sensitivities of 1.29 and 1.75 µA µmol L^{-1} cm^{-2}, respectively. Selectivity studies demonstrated well-resolved oxidation peaks for ascorbic acid (AA) (−0.07 V), DA (+0.20 V), and uric acid (UA) (+0.57 V), confirming effective discrimination of DA in the presence of interferents. These results highlight the potential of 3D electrodes as cost-effective platforms for point-of-care DA monitoring.

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GR45CO15 sensor for detecting DA.

Agradecimentos/Acknowledgments

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Development of a prototype using additive manufacturing technology for monitoring gases produced during the study of water electrolys.

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Palavras Chave:*Additive manufacturing, 3D printing, water electrolysis, sensors of dissolved gases.,Additive manufacturing,3D printing,water electrolysis,sensors of dissolved gases*

Highlights

Printing a 3D electrochemical cell H type prototype.

Optimize the cell prototype.

Monitoring hydrogen and oxygen produced by water electrolysis.

Use sensors for monitoring dissolved gases.

Resumo/Abstract

The global decarbonization effort is one of many efforts to compliment with the Sustainable Development Goals (SGDs) and in the last decade the hydrogen was recognized as a key in energy carrier for a sustainable future. However, cost-effective hydrogen production technologies require a lot of research and development in the actual setting.[1] Between the requirements, reliable and precise methods for gas quantification during electrochemical processes are essential for catalyst evaluation and performance optimization. Dissolved gas microsensors provide fast and sensitive measurements, but the existing standardized electrochemical cells aren't specifically designed to integrate these sensors with high reproducibility available. In this context, additive manufacturing as Fused Deposition Modeling (FDM) is used for designing and printing prototypes with a low cost and versatility.[2] This work presents the development of a 3D-printed H-type electrochemical cell designed for the integration of Unisense dissolved gas microsensors. The system allows for in situ quantification of hydrogen and oxygen during water electrolysis, ensuring proper sensor positioning, compartment isolation, and experimental reproducibility. It realized an analysis variation of some parameters such as concentration of solution, electrodes, and design of the 3D cell. Previous results with the first design presentation of Faradaic Efficiencies of 49,57% for Hydrogen and 58,77% for Oxygen in the system of FTO and KOH 1M. After that, some catalysis of the group is used for quantification. The proposed design offers a low-cost, adaptable, and reproducible platform for evaluating catalytic hydrogen production under laboratory conditions. The developed cell contributes to improving analytical reliability in electrocatalysis studies and supports advances in sustainable hydrogen production technologies.



Electrochemical Cell. (a) and (b) Design of an electrochemical cell and (c) Printed Cell.

Agradecimentos/Acknowledgments

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DEVELOPMENT OF A WEARABLE HYDROGEL-BASED ELECTROCHEMICAL SENSOR FOR SOLID-STATE DETECTION OF CARBENDAZIM IN FRUITS

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Palavras Chave:*Electrochemical sensor; agarose; pesticide; wearable device; solid-state detection.,An innovative hydrogel-integrated screen-printed electrochemical sensor enables direct extraction and detection of carbendazim from solid samples*

Highlights

An innovative hydrogel-integrated screen-printed electrochemical sensor enables direct extraction and detection of carbendazim from solid samples

Resumo/Abstract

Population growth has increased pesticide use in agriculture, raising risks to health and environment. Among pesticides most frequently detected in Brazil, carbendazim stands out and, although banned by ANVISA in 2022 due to toxicity, continues to be reported, reinforcing need for monitoring. In Brazil this control is performed by Pesticide Residue Analysis Program in Food (PARA), which relies on costly instrumentation and limits rapid analyses. Wearable electrochemical sensors represent na alternative, but most depend on liquid electrolytes and require laborious preparation for solid samples. Screen-printed electrodes integrated with hydrogels acting simultaneously as electrolyte and extraction phase were therefore investigated. Carbendazim oxidation was characterized in aqueous medium by cyclic and square-wave voltammetry, showing best response at pH 4 and oxidation potential near 0.7 V, and this pH was adopted in subsequent experiments. Under this condition, agarose hydrogels (1–3% m/m) were prepared in Britton–Robinson buffer (pH 4) containing 0.01 mol L^{-1} NaCl by dispersing agarose in buffered solution followed by microwave heating for about 20 seconds in 5 second intervals until dissolution, casting and cooling to obtain solid material. NaCl systems showed lower water loss and better mechanical stability, while sucrose-only compositions (3% and 30%) dehydrated more. To evaluate extraction from solid surface, circular polietileno tereftalato (PET) substrates received successive aliquots of carbendazim solution dried between additions until total volume of 5 µL was reached. Contaminated PET substrate was placed in contact with 2% agarose 0.01 mol L^{-1} NaCl hydrogel on electrode, generating voltammetric signal that increased until stabilization after approximately 20 minutes, demonstrating extraction. Future studies will evaluate mixed sucrose and NaCl compositions, other hygroscopic salts, electrode modification, analytical optimization and calibration curves.

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Effect of biochar and temperature on nickel electrodeposition in different deep eutectic solvents

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Palavras Chave:*Electrodeposition,Deep eutectic solvents,Nucleation,Biochar*

Highlights

Biochar and temperature influenced the electrocrystallization of nickel in a magnetic eutectic solvent on 1020 carbon steel, promoting the transition between progressive and instantaneous nucleation.

Resumo/Abstract

Here we study the nucleation and growth of Ni^{2+} on 1020 carbon steel at 23 °C and 45 °C without and with biochar (BCP). Solutions containing choline chloride (ChCl), ethylene glycol (EG), urea (U) and $NiCl_2$, called 1ChCl:2EG:1NiCl2 and 1ChCl:2U:1NiCl2, were prepared. At 23 °C, −0.3 V was applied for 30 s followed by step potentials between −0.46 V and −0.51 V for 60 s. The results were analyzed according Scharifker and Hills' model with D = 2.2×10−¹¹ cm² s−¹ and nucleus formation rate (AN∞) varying between 4.5×10⁷ cm² s−¹ and 8.2×10⁸ cm² s−¹ and D = 1.4×10−¹¹ cm² s−¹ and AN∞ varying between 1.2×10⁸ cm² s−¹ and 3.8×10⁹ cm² s−¹ for 1ChCl:2EG:1NiCl2 and 1ChCl:2U:1NiCl2, respectively. Adding biochar at 23 °C, 1ChCl:2EG:1NiCl2 + 500 mg BCP showed progressive nucleation with D = 1.1×10−¹² cm² s−¹ and AN∞ varying from 1.4×10⁸ cm² s−¹ to 1.3×10⁹ cm² s−¹ and 1ChCl:2U:1NiCl2 + 500 mg BCP showed instantaneous nucleation with D = 1.2×10−¹² cm² s−¹ and number of formed nuclei (N) varying from 1.2×10⁵ cm² s−¹ to 2.4×10⁵ cm² s−¹, respectively. Now, analyzing the influence of temperature, experiments at 45 °C were carried out, in which ChCl:2EG:1NiCl2 showed instantaneous nucleation with D = 3.2×10−¹² cm² s−¹ and N varying from 6.9×10⁵ cm² s−¹ to 2.2×10⁶ cm² s−¹ and 1ChCl:2U:1NiCl2 showed progressive nucleation and D = 5.8×10−¹² cm² s−¹ and AN∞ ranging from 9.2×10⁹ cm² s−¹ to 3.5×10¹⁰ cm² s−¹, respectively. Combining temperature increase with addition of biochar, 1ChCl:2EG:1NiCl2 + 500 mg BCP and 1ChCl:2U:1NiCl2 + 500 mg BCP showed instantaneous nucleation with D = 2.6×10−¹² cm² s−¹ and N ranging from 4.2×10⁵ cm² s−¹ to 1.4×10⁶ cm² s−¹ and D = 3.5×10−¹² cm² s−¹ and N ranging from 1.3×10⁶ cm² s−¹ to 2.5×10⁶ cm² s−¹, respectively. Thus, it is concluded that the addition of biochar, associated with increased temperature, exerted a significant influence on the electrocrystallization of nickel, promoting the transition between the progressive and instantaneous nucleation nucleation.

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Effect of Nanostructuring of Au Electrodes on the Electrical Double Layer

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Palavras Chave:*Electrical double layer; Gold electrodes; Nanostructuring; Differential capacitance; Potential of zero charge*

Highlights

Pulsed potentials modify gold electrodes surface.
The properties of the EDL were evaluated by capacitance measurements.
Nanostructuring influences the EDL structure.

Resumo/Abstract

Classical models of the electrical double layer are based on classical physics mean-field approximations and assume ideal, flat, and infinite electrodes, often represented by mercury surfaces. Although fundamental, such approximations become limited when confronted with the real conditions of electrochemical and surface chemistry applications. In this context, this work seeks to contribute to the understanding of the interfacial region between nanostructured gold electrodes and electrolytes. Initially, the electrode nanostructuring procedure was optmized based on factorial designs considering, as input variables, potential perturbations in triangular waveforms, observed to be inefficient, and pulsed waveforms, which were more effective. The optimized potential window was between the reduction of gold oxides and oxygen evolution. The time fixed at each potential did not influence the roughening, while it showed a linear dependence on the number of repetitions. Electronic spectroscopy investigation showed a response in the Au plasmonic band in the green region. Variations in the properties of the EDL were analyzed from the double-layer capacitance as a function of potential and electrolyte concentration, using low-amplitude cyclic voltammetry and differential capacitance. The latter showed greater accuracy in determining the potential of zero charge.

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Effects of variation of the geometric area of Au electrodes as a bifurcation parameter for the SO2 oxidation reaction

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Palavras Chave:*Green hydrogen,Renewable energy,Geometric area,Roughness,Bifurcation parameter*

Highlights

Production of green hydrogen from the oxidation of SO_2.
Variation in the geometric and surface area of the gold electrode.
Consumption of the atmospheric pollutant SO_2.

Resumo/Abstract

The environmental damage resulting from the use of fossil fuels and the significant production of polluting gases produced in this process is becoming increasingly urgent. The generation of green hydrogen is a renewable energy storage process with high potential, but it is limited by the high energy barrier of the oxygen release reaction. Replacing this oxidation reaction with other processes such as the oxidation of SO_2, a highly toxic air pollutant, is of great interest, because it has a low standard potential, a low activation barrier on Au, as well as high currents, and generates H_2SO_4 as the main product.
The influence of surface area, through the variation of roughness, as well as the geometric area of the electrode, both parameters for the SO_2 oxidation reaction, were analyzed by kinetic investigations with classical electrochemical techniques, in addition to the influence of the increase in area, real and geometric, on kinetic instabilities.

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Electrocatalytic Nitrate Reduction to Ammonia Using Two-Dimensional Ti3C2Tx MXene

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Palavras Chave:*Ammonia electrosynthesis, MXenes, $Ti_3C_2T_x$, Electrocatalysis*

Highlights

This study synthesized $Ti_3C_2T_x$ MXene as a promising catalyst for electrochemical nitrate-to-ammonia reduction, showing ~55% Faradaic efficiency and yield rates exceeding 600 µmol h^{-1} cm^2.

Resumo/Abstract

The electrochemical reduction of nitrate (NO_3-) to ammonia (NH_3) has emerged as a promising, environmentally sustainable strategy for decentralized ammonia production, offering a low-impact alternative to the conventional Haber–Bosch process. This approach converts residual nitrate into value-added chemicals using renewable electricity. However, the nitrate reduction reaction (NO_3RR) remains limited by low selectivity and catalytic efficiency with current materials. MXenes have attracted increasing attention for their high electrical conductivity, layered structure, and tunable surface chemistry. In this work, pristine $Ti_3C_2T_x$ MXene was synthesized via HF-assisted chemical exfoliation and evaluated as an electrocatalyst for NO_3RR in alkaline media. The material was characterized by XRD, HRTEM, SEM-EDS, AFM, Raman, and UV–Vis spectroscopy, confirming the formation of uniform few-layer films with an average thickness of approximately 1 nm. Electrochemical behavior was investigated by cyclic voltammetry, which showed a marked increase in cathodic current density in the presence of nitrate, consistent with NO_3RR activity. Chronoamperometry between −0.3 and −0.6 V vs. RHE demonstrated enhanced ammonia production, with Faradaic efficiencies above 55% at −0.6 V and yield rates exceeding 600 µmol h^{-1} cm^2. These results highlight the electrocatalytic potential of pristine $Ti_3C_2T_x$ for nitrate-to-ammonia conversion, while underscoring the importance of expanding the MXene compositional space. Investigating alternative active metals within the MXene framework may enable the rational design of superior NO_3RR catalysts, combining the advantages of two-dimensional architectures with intentionally steered reaction pathways through multiple active sites.

Agradecimentos/Acknowledgments

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Electrocatalytic N_2 Reduction by Improving the Electrolytic Conditions Using Water in Salt Electrolytes (WISE)

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Palavras Chave:*nitrogen electrochemical reduction (eNRR),ammonia electrosynthesis,water-in-salt electrolyte (WISE),silver nanoparticles (Ag NPs),zeolitic imidazolate framework (ZIF).*

Highlights

Enhancement of eNRR performance through rational tuning of Water-in-Salt Electrolytes (WISE). Correlation of electrolyte physicochemical properties with N_2 solubility, free-water availability, and pH.

Resumo/Abstract

Ammonia electrosynthesis is emerging as a promising alternative to the Haber-Bosch (HB)[1]process. Such interest arises from the fact that the HB process requires high temperature and pressure, whereas electrocatalytic processes operate under mild conditions. However, challenges related to the low solubility of N_2, pH and fraction of free water leading side reactions such as hydrogen evolution reaction (HER)[2] are the main challenges that needs to be overcome. In this work, a catalyst composed of zeolitic imidazolate framework (ZIF)[3] combined with Ag nanoparticles (Ag NPs) giving Ag@ZIF-8 was used as model to understand the physicochemical properties of different water in salt electrolytes (WISE)[4] towards the electrochemical N_2 reduction reaction (eNRR)[5]. Our comprehensive experimental results, corroborated by theoretical calculations demonstrated that the N_2 solubility is lower under 12*m*(m = mol kg^{-1})(pH = 6.0 and 34.5% free H_2O) and 15*m*(pH = 4.3 and 18% free H_2O) LiTFSI compared to the 28*m*(pH = 10.6 and 0% free H_2O) CH_3COOK. Such behavior reveals that the nature and concentration of the electrolytes directly govern the solubility of N_2 and availability of water in the system,**Figure 1**. To validate these findings, controlled potential electrolysis in all the different WISEs of LiTFSI and CH_3COOK were carried out, showing the best performance achieved under ultra-high salt concentration 28*m*CH_3COOK, FE 46.4% at 0.0 V*vs*RHE and ammonia yield rate of 2993.53 µg $mgAg^{-1}$ h^{-1}.

The results obtained are consistent with the predicted tailored physicochemical properties of the WISE electrolytes, offering an alternative strategy to enhance ammonia electrosynthesis by tunning the electrolytic conditions.

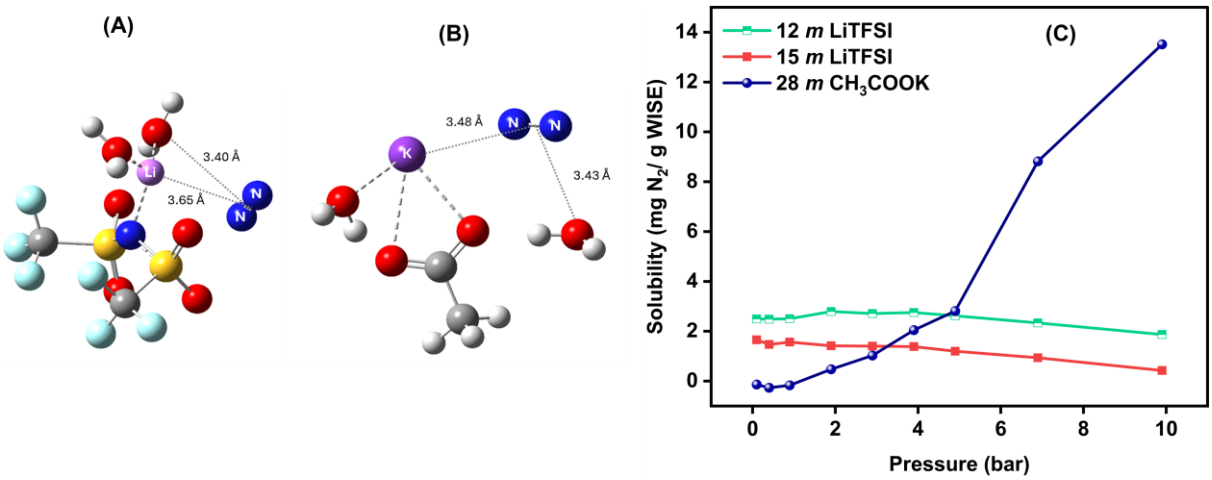


Figure 1. (A,B) Structures of the WISEs with an N_2 molecule.(C) N_2 solubility in the different WISEs

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Electrochemical characterization of acetate-based Water-in-Salt Electrolytes (WiSE) for zinc-air batteries

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Palavras Chave:*Zinc-air (Zinc-O2) batteries,Zn-air (Zn-O2),Water-in-Salt Electrolyte,WiSE*

Highlights

Acetate-based WiSE electrolytes for rechargeable Zn–air batteries Wide electrochemical window and stable Zn redox behavior Microelectrodes used to estimate diffusion limits

Resumo/Abstract

Zinc–air ($Zn–O_2$) batteries have emerged as a promising low-cost and lower-environmental-impact alternative for energy storage when compared to lithium-ion technologies. However, challenges such as dendrite formation, parasitic reactions, and limited electrolyte electrochemical stability still hinder their reversible operation. In this context, highly concentrated aqueous electrolytes of the Water-in-Salt (WiSE) type have been investigated as a strategy to expand electrochemical stability and modulate interfacial processes.

This work investigates the electrochemical behavior of acetate-based WiSE electrolytes composed of zinc acetate and potassium acetate at different concentrations, targeting their application in rechargeable $Zn–O_2$ systems. The electrochemical stability window was determined by linear sweep voltammetry under an oxygen atmosphere, showing a stability range of approximately 2.5 V (0.0–2.5 V vs. Zn/Zn^{2+}), as presented in Figure 1a.

Zinc redox behavior was evaluated by cyclic voltammetry using glassy carbon electrodes, enabling simultaneous assessment of how electrolyte concentration affects zinc deposition and stripping processes. The voltammetric profiles display characteristic redox features and good reversibility within the investigated potential range, together with concentration-dependent changes in current density and anodic/cathodic hysteresis (Figures 1b and 1c).

These differences are associated with variations in ionic mobility, viscosity, and mass-transport regime in superconcentrated media, which directly influence deposition stability and metallic deposit morphology. In addition, microelectrodes were fabricated and employed for transport analysis, allowing estimation of diffusion coefficients and evaluation of kinetic limitations under WiSE conditions.

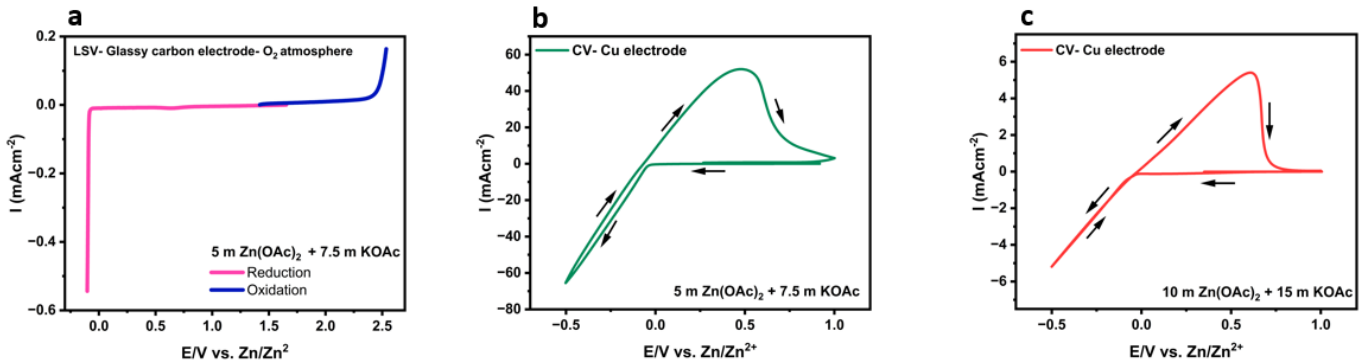


Figure 1. LSV (a) and CV (b,c) of $Zn(OAc)_2$/KOAc WiSE at 5/7.5 m and 10/15 m

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Electrochemical Characterization of Mushroom Waste-Derived Biochar for Sensing Applications

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Palavras Chave:*biochar,electrochemical,cyclic voltammetry,electroanalysis,sensors*

Highlights

Mushroom waste-derived biochar shows promising electrochemical properties, highlighting its potential as a sustainable material for electroanalytical sensors.

Resumo/Abstract

The growing demand for sustainable analytical devices has driven the reuse of biomass waste for the synthesis of functional carbon-based materials. In this context, biochar stands out as a promising surface modifier for electrochemical sensors due to its high porosity and abundance of oxygenated functional groups, which facilitate charge transfer. This study presents the development and electrochemical characterization of a carbon paste electrode (CPE) modified with biochar derived from mushroom cultivation waste. The precursor material was pyrolyzed and processed to a nanometric particle size (150–250 nm) to maximize the electroactive surface area. Sensors were prepared by mechanically homogenizing graphite powder, biochar (10% and 20% w/w), and castor oil as a binder for 20 minutes using a mortar and pestle. Electrochemical characterization was performed using cyclic voltammetry in a 5 mmol L^{-1} ferri/ferrocyanide solution in 0.1 mol L^{-1} KCl. Results showed that the incorporation of biochar significantly increased current density. The sensor containing 20% biochar exhibited peak currents of approximately 710 µA, considerably higher than the 392 µA recorded for the 10% formulation and significantly higher than the 121 µA observed for the pure CPE (all at 400 mV s^{-1}), indicating substantial improvements in electron transfer kinetics and mass transport. The linear relationship between peak current and the square root of the scan rate confirmed a diffusion-controlled process. In conclusion, mushroom waste-derived biochar proves to be a low-cost, highly sensitive, and environmentally friendly material, showing strong potential for detecting environmentally and pharmacologically relevant analytes such as heavy metals and organic contaminants.



Biochar produced from mushroom waste.

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Electrochemical Degradation of Diuron at Environmentally Relevant Conditions

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Palavras Chave:*Diuron, Electrochemical oxidation, Boron-doped diamond (BDD), Low-conductivity, Decentralized wat,Diuron, Electrochemical oxidation, Boron-doped diamond (BDD), Low-conductivity, Decentralized water treatment.,Diuron,Electrochemical oxidation,Boron-doped diamond (BDD),Low-conductivity,Decentralized water treatment*

Highlights

BDD anodes enabled efficient degradation under conditions mimicking some domestic wastewater.

Increasing current density significantly enhaced degradation kinetics due to higher •OH generation.

Resumo/Abstract

Diuron is an herbicide widely used in Brazil, and its occurrence in aquatic environments raises environmental and human health concerns. Conventional water treatment processes are ineffective in removing herbicides, highlighting the need for appropriate treatment technologies. In this context, electrochemical oxidation (EO) has emerged as an environmentally friendly alternative due to its operational simplicity. In this study, the electrochemical oxidation of diuron was investigated under environmentally relevant conditions using a boron-doped diamond (BDD) anode at laboratory scale. The solution conductivity was kept low (1.78 mS cm^{-1}) to simulate conditions found in domestic wastewater. Diuron concentration was monitored by HPLC, and the effects of current density (j), initial diuron concentration, and initial pH were systematically evaluated. Increasing j accelerated diuron degradation due to the enhanced generation of hydroxyl radicals, the main species responsible for diuron oxidation. The process was effective over the entire concentration range studied (0.25–5.0 mg/L). However, at very low concentrations, degradation rates decreased due to mass transport limitations. For example, the observed rate constant (kobs) decreased from 0.203 min^{-1} at 0.50 mg/L to 0.0777 min^{-1} at 0.25 mg/L indicating diffusion-controlled conditions. The fastest degradation was achieved at pH 3, whereas higher pH values led to reduced oxidation rates due to the lower reactivity of hydroxyl radicals. Nevertheless, comparable degradation rates were observed at pH 7 and 10, demonstrating that EO can operate efficiently under neutral and alkaline conditions. Overall, the results confirm that electrochemical oxidation is a promising approach for the removal of environmentally relevant concentrations of herbicides under conditions representative of real waters, reinforcing its potential application in decentralized water treatment systems.

Agradecimentos/Acknowledgments

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Electrochemical Detection of Cannabidiol Using Carbon-Based Electrodes Supported by DFT Insights.

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Palavras Chave:*Cannabidiol, Electroanalysis, Carbon-based electrodes, Density functional theory,Cannabidiol,Electroanalysis,,Carbon-based electrodes,,Density functional theory*

Highlights

Electrochemical oxidation of CBD investigated using carbon-based electrodes. DFT dual descriptor identified oxygen atoms as oxidation sites.

Resumo/Abstract

Cannabidiol (CBD) is a bioactive compound widely used in pharmaceutical formulations, whose routine quantification still relies mainly on chromatographic techniques. In this context, electrochemical methods represent an attractive alternative due to their rapid response, low cost, and operational simplicity. In this work, the electrochemical behavior of CBD was investigated using carbon-based electrodes, and a sensitive electroanalytical method for its determination was proposed. Density functional theory (DFT) calculations were employed to support the interpretation of the electrochemical results. The molecular geometry of CBD was optimized using the BP86 functional combined with the Def2-TZVPPD basis set and D3BJ dispersion corrections within an implicit solvent model. Analysis of the dual descriptor indicated that both oxygen atoms are the most susceptible molecular sites toward oxidation. Experimentally, cyclic voltammetry performed at a glassy carbon electrode revealed an irreversible oxidation peak at approximately +0.4 V (vs. Ag/AgCl(sat.)). The shift of the oxidation potential with pH suggested the involvement of protons in the electrochemical process. Differential pulse voltammetry showed excellent analytical performance under optimized supporting electrolyte conditions, with a linear concentration range from 0.36 to 11.52 mg L^{-1} and a theoretical limit of detection of 0.12 mg L^{-1}. Recovery assays yielded an average value of 98% (n = 3), and the determination of CBD in commercial oral oil samples showed good agreement with the reference HPLC-UV method. The proposed electroanalytical approach demonstrates strong potential for the routine sensing of CBD and for quality control applications in pharmaceutical products.

Agradecimentos/Acknowledgments

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Electrochemical Oxidation of Lignin: Mechanism and Kinetics Investigation

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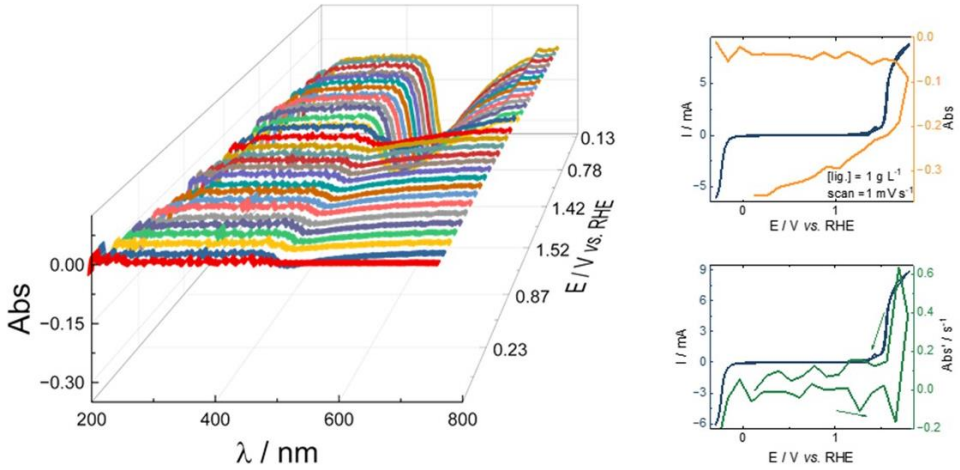
Palavras Chave:*Biomass valorization,Electrochemical Lignin Oxidation,Electrocatalysis,Electrobiorefinery*

Highlights

Multi-step mechanism was observed; Intermediates adsorption was characterized by Frumkin's isotherm;*In situ*electronic spectroscopy showed reversibility of the process.

Resumo/Abstract

The search for sustainable alternatives has driven the study of lignocellulosic biomass as a renewable source of energy and feedstock materials. Lignin, a frequent industrial and agricultural residue, is a potential source of high value-added aromatic compounds. However, due to its complex structure, its depolymerization is costly and difficult. Electrocatalysis emerges as an energetically efficient and easily controllable strategy for its oxidative cleavage into carbonylated monophenols. This study employs electrochemical methods to investigate the kinetics and mechanisms of lignin electrochemical oxidation in alkaline medium, on nickel electrodes. Voltammetric studies indicate the presence of adsorbed intermediates, through pseudocapacitive behavior and kinetic limitations, as demonstrated by Tafel-type plots. Adsorption was also investigated using isotherms, revealing Frumkin behavior. In situ electronic spectroscopy in transmittance configuration suggested the presence of intermediates and process reversibility. After the oxidation, the organic soluble species were characterized by vibrational spectroscopy, which showed structural changes, as the diminish of Cα-Cβ related band.



Spectroelectrochemical investigation on LEOR

Agradecimentos/Acknowledgments

FAPESP (#2019/22183-6, #2020/15230-5, #2022/06405-1 e #2024/13277-5), ao RCGI/USP & Shell Brasil, e à ANP.

Electrochemical Reduction of Nitrite to Nitric Oxide by Tripodal Amine Based Copper Complexes for Biomedical Applications

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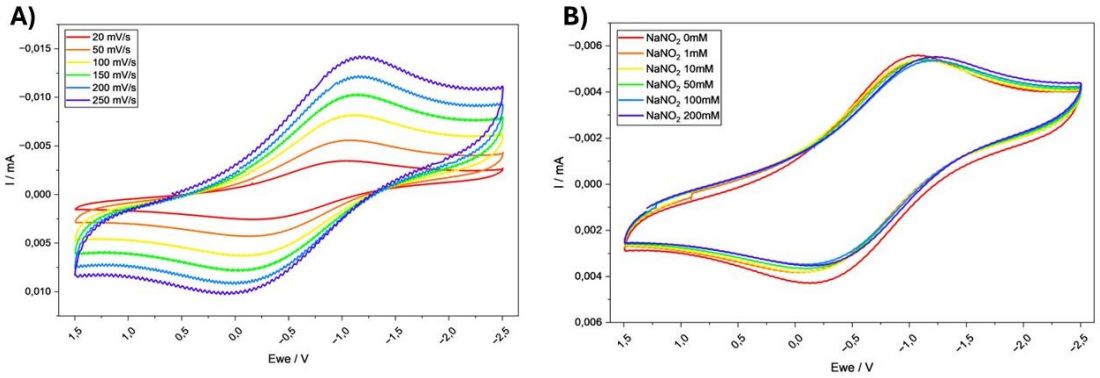
Palavras Chave:*Electrochemistry,Nitric Oxide,Copper Complexes,Biomimetics,Tripodal Amine Ligands*

Highlights

Design and synthesis of tripodal amine-based copper complexes with tunable redox properties; Electrochemical reduction of nitrite to nitric oxide for potential biomedical applications.

Resumo/Abstract

Nitric oxide (NO) is a key endogenous signaling molecule that plays a central role in physiological functions such as vascular regulation, immune defense and prevention of platelet aggregation. The integration of NO-releasing system into intravenous (IV) catheters has emerged as a potential strategy to reduce complications related to thrombosis and bacterial colonization in vascular access devices. In this context, our research focuses on the development of IV catheters capable of generating NO through the electrochemical reduction of NO_2^-, a stable, non-toxic, and economically viable NO source, mediated by newly designed Cu(II)-ligand catalysts. Initially, six Cu(II)-based complexes were examined, including Copper BMPA- and BEPA- Carboxylate Complexes. While improvements in catalyst stability, NO release rates, and antimicrobial performance were achieved, challenges persisted, particularly the oxygen sensitivity associated with the negative reduction potentials of these systems. NO generation experiments monitored using a nitric oxide analyzer (NOA) showed that the introduction of gas mixtures containing 3% and 10% O_2, compared to an inert N_2 atmosphere, results in a significant decrease in detected NO flux. To overcome this limitation, ligand frameworks were modified by replacing pyridine units with quinoline moieties, inspired by studies in copper–oxygen chemistry (JACS, 1993, 9506). Furthermore, a new family of ligands incorporating pyrazole and quinoline groups was synthesized and coordinated to Cu(II) using different counterions, including acetate, perchlorate, and sulfate.
The resulting complexes were characterized by spectroscopic methods, and their electrochemical behavior was evaluated by cyclic voltammetry, showing a stable redox complex (Fig A), and the coordination of NO_2^- to the copper center by the shift of the reduction potential to more negative values (Fig B). These preliminary results indicate promising potential for electrochemical NO generation.



Cyclic voltammetry of 1mM Cu-complex. (A) Scan rate dependence study and (B) $NaNO_2$ Titration

Agradecimentos/Acknowledgments

The author acknowledges Prof. Nicolai Lehnert, Dr. Nabhendu Pal and Arup Sarkar for supervision and scientific guidance, the Lehnert research group for valuable discussions, and the University of Michigan for research infrastructure.

Electrochemistry and Antioxidant Activities of Substituted Furanyl Nitrone: The Role of the Nitro Group

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Palavras Chave:*Nitronas, Eletroquímica orgânica, Voltametria cíclica, Mecanismo redox.*

Highlights

The electrochemical and antioxidant behavior of substituted furanyl nitrone was investigated. Nitrones' antioxidant capacity (AO), despite being very low, correlates with their oxidation profiles.

Resumo/Abstract

As nitronas são antioxidantes sintéticos com potencial terapêutico (1–2), destacando-se a LQB-303 pela potente atividade tripanocida, alta seletividade e baixa toxicidade (3). No presente trabalho, foi investigado o comportamento eletroquímico e antioxidante de nitronas para obter dados sobre seu mecanismo redox a fim de corroborar, explicar ou prever os mecanismos moleculares de ação biológica (4). Voltamogramas cíclicos (VCs) foram registrados em eletrodo de carbono vítreo (ECV) em meio aprótico (acetonitrila + 0,1 M TBAPF6) a fim de mimetizar os ambientes biológicos lipofílicos. A avaliação da capacidade antioxidante foi realizada pelos métodos espectroscópicos de FRAP (poder antioxidante de redução de íons ferro) e capacidade antioxidante sequestradora frente ao radical DPPH•. O precursor aldeído original**5NBFAL**foi estudado eletroquimicamente nas mesmas condições. Os VCs de**LQB-109**exibem duas ondas catódicas irreversíveis em −2,04 V e − 2,19 V (Fig.1A), relacionadas a uma redução de quatro elétrons para hidroxilamina (Fig.1B). Duas ondas anódicas apareceram em +1,32 V e +1,53 V (Fig.1C). A primeira captação de elétrons para**LQB-569**ocorre no grupo nitroaromático, seguida por reduções para dar um nitroso mais eletrofílico, propenso a dimerizar e formar derivados azoxi redutíveis, juntamente com a redução de nitrona, em um processo total de 10 elétrons (Fig.1E). Uma onda anódica irreversível em +1,45 V aparece, relacionada à oxidação da nitrona (Fig.1D). A capacidade antioxidante (AO) das nitronas se correlaciona com seus perfis de oxidação, e aquelas capazes de oxidar mais facilmente tiveram melhores resultados na eliminação de DPPH• e FRAP. LQB-569 mostrou baixa CA, devido à presença do grupo retirador de elétrons, refletindo a parte oxidativa dos VCs.**REFERÊNCIAS:**[1] Rosselin et al., Curr. Top. Med. Chem., 2017; [2] Costa et al., Bioorg. Med. Chem., 2015; [3] Macedo et al., Front. Microbiol., 2021; [4] Santos et al., ChemElectroChem, 2025.

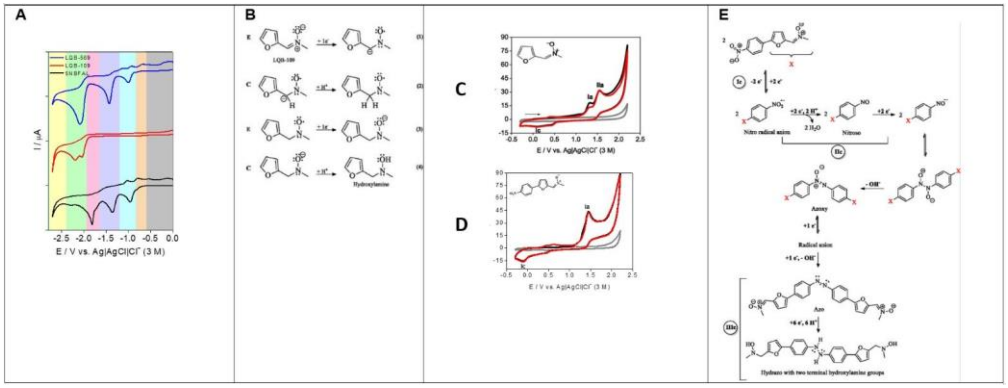


Figura 1. (A) VCs catódicas. (B) Redução LQB-109. (C–D) VCs anódicas. (E) Mecanismo LQB-569.

Agradecimentos/Acknowledgments

FAPEAL, CNPQ, CAPES, RENORBIO, INCTBIO, UFAL and PET Química.

Eletrodo fotoeletroquímico baseado em papel de grafeno modificado com filmes finos de $BiVO_4$ para detecção de H_2O_2

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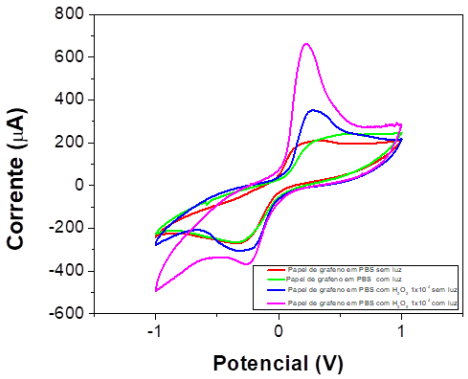
Palavras Chave:*Papel de grafeno,Vanadato de bismuto ($BiVO_4$),Fotoeletroquímica,Voltametria cíclica,Peróxido de hidrogênio*

Highlights

Graphene paper electrodes modified with $BiVO_4$ thin films
Photoelectrochemical response via semiconductor photoactivation
Photoassisted electrochemical detection of H_2O_2

Resumo/Abstract

A detecção de peróxido de hidrogênio (H_2O_2) é de grande relevância em análises ambientais, biomédicas, industriais e de segurança alimentar, em função de seu papel como agente oxidante e intermediário em diversos processos químicos e biológicos (Chen*et al.*, 2012). Nesse contexto, sensores fotoeletroquímicos (PEC) têm atraído crescente interesse por apresentarem baixo custo, alta sensibilidade, rápida resposta e simplicidade operacional. Em sistemas PEC, a iluminação do material semicondutor promove a geração de pares elétron–lacuna, que participam de processos de transferência de carga na interface eletrodo/solução, convertendo o estímulo luminoso em um sinal eletroquímico mensurável (Li*et al.*, 2019). Entre os semicondutores empregados, o vanadato de bismuto ($BiVO_4$) destaca-se por sua estabilidade química e propriedades fotoativas favoráveis à separação de cargas. Assim, este trabalho tem como objetivo desenvolver e avaliar um eletrodo fotoeletroquímico baseado em papel de grafeno modificado com filmes finos de $BiVO_4$ para a detecção de H_2O_2. O eletrodo de trabalho foi constituído por papel de grafeno, associado a contraeletrodo e eletrodo de pseudo-referência impressos com tinta de carbono, sendo este último modificado com Ag/AgCl. A modificação foi realizada por deposição, via*drop casting*, de 5 µL de uma suspensão de $BiVO_4$, seguida de secagem à temperatura ambiente por 12 h. Os ensaios eletroanalíticos foram conduzidos por voltametria cíclica em solução tampão fosfato (PBS, pH 7,0) contendo 1,0 × 10^{-4} mol L^{-1} de H_2O_2, sob ausência e presença de estímulo luminoso. Observou-se o deslocamento do potencial de pico de 0,265 V para 0,218 V na condição fotoassistida, acompanhado de aumento das correntes faradaicas, indicando redução do sobrepotencial e melhoria da cinética de transferência de carga. Os resultados demonstram o potencial do eletrodo para aplicações eletroanalíticas fotoassistidas.Parte superior do formulário



Voltamogramas cíclicos em PBS e PBS com H_2O_2 (1,0×10 $^{-4}$ mol L $^{-1}$), com e sem estímulo luminoso.

Agradecimentos/Acknowledgments

Instituto de Ciênica, Engenharia e Tecnologia da Universidade Federal dos Vales do Jequitinhonha e Mucuri - UFVJM; Fundação de Amparo à Pesquisa do Estado de Minas Gerais - FAPEMIG pelo projeto APQ-00607-22; CAPES.

Eletro-refinaria em meios salinos: co-geração de hidrogênio verde e oxidantes em sistemas eletroquímicos sustentáveis

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Palavras Chave:*eletrólise híbrida, águas residuais salinas,Eletro-refinaria,Águas residuais salinas,Hidrogênio verde*

Highlights

Solar-driven electro-refinery enables simultaneous green H_2 production and active chlorine generation from saline wastewater.

Resumo/Abstract

A crescente demanda por rotas sustentáveis de produção de hidrogênio (H_2) impulsiona o desenvolvimento de sistemas eletroquímicos capazes de integrar geração de energia limpa e tratamento de efluentes. Neste contexto, este trabalho apresenta o conceito de eletro-refinaria em meios salinos, baseado em um sistema de eletrólise híbrida alimentado por energia solar, projetado para a co-geração de H2 e oxidantes ativos à base de cloro (ClO^-) a partir de efluentes salinos reais. O reator eletroquímico foi otimizado por meio da incorporação de um dosador de cloreto, permitindo maior controle da cinética de formação de oxidantes. A análise cinética revelou comportamento de pseudo-primeira ordem para a eletrogeração de ClO^-, tanto em soluções sintéticas quanto em efluentes industriais. O sistema modificado apresentou aumento expressivo na eficiência de conversão, elevando em cerca de 25%, além de produzir concentrações de ClO^- até 19 vezes superiores às obtidas em configurações convencionais. A produção de H_2 seguiu tendência linear de acordo com a Lei de Faraday, com desvios médios de proximadamente 17% em matrizes reais, evidenciando boa previsibilidade eletroquímica mesmo em condições complexas. O consumo energético específico variou entre 0,171 e 0,990 kWh kg^{-1} de H_2, dependendo da densidade de corrente e da concentração de cloreto, indicando viabilidade energética competitiva. Adicionalmente, os custos de tratamento (US$ 0,31–2,63 m^{-3}) situam-se na faixa de tecnologias convencionais, reforçando o potencial de aplicação industrial. Os resultados demonstram que a eletro-refinaria em meios salinos representa uma estratégia promissora para integrar produção de energia, geração de oxidantes e remediação ambiental em um único sistema. Essa abordagem contribui diretamente para os princípios da economia circular, ao transformar efluentes em recursos, reduzindo a dependência de água purificada e ampliando a sustentabilidade de processos eletroquímicos.

Agradecimentos/Acknowledgments

Financial support from the Human Resources Training Program of the National Agency of Petroleum, Natural Gas and Biofuels (PRH-ANP), Process No. 2025/18303-7. CNPq (408110/2022-8, 421313/2023-4).

Engineering Closed Pores in Hard Carbons via Covalent Organic Frameworks for Sodium-Ion Batteries

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Palavras Chave:*Covalent organic framework, hard carbon, SIBs, closed pores, batteries*

Highlights

COFs enabled closed-pore formation in self-supporting hard carbon electrodes. 2.5 wt% COF increased ICE from 59% to 92%. Plateau contribution rose from 45% to 65%, improving Na^+ storage.

Resumo/Abstract

The search for alternatives to lithium-ion batteries has intensified due to lithium scarcity and the high costs associated with its extraction and processing. In this context, sodium-ion batteries (SIBs) have emerged as a promising option, owing to the chemical similarity between Li^+ and Na^+ ions and the possibility of reusing existing battery manufacturing infrastructure. One of the main challenges in SIBs is the development of efficient anode materials, with hard carbon currently considered the state-of-the-art.

Hard carbon is a non-graphitizable material, even at temperatures above 3000 °C, and stores sodium through a combination of mechanisms involving semi-graphitic domains, structural defects, and porosity. Among these, Na^+ intercalation into semi-graphitic layers is responsible for the low-potential plateau capacity and is strongly associated with the presence of closed pores. Therefore, strategies that promote closed-pore formation are key to improving electrochemical performance.

In this work, a covalent organic framework (COF) synthesized via mechanochemical methods was incorporated into self-supporting hard carbon electrodes as a closed-pore-forming agent. The addition of small amounts of COF significantly improved the electrochemical performance, increasing the initial coulombic efficiency (ICE) from 59% for pristine hard carbon to 92% for COF-modified electrodes. In addition, the reversible capacity increased from 148 to 257 mAh g^{-1}, demonstrating enhanced sodium and energy storage. Moreover, the contribution of the plateau region increased from 45% to 65%, indicating more efficient Na^+ storage via intercalation. In contrast, the reference HC electrode exhibited a dominant slope contribution, consistent with sodium storage governed by surface adsorption. These results demonstrate that COF incorporation is an effective strategy to tailor the pore structure of hard carbon and enhance its performance as an anode material for sodium-ion batteries.

Agradecimentos/Acknowledgments

The authors are grateful for the financial support provided by the São Paulo Research Foundation (FAPESP, grants No. 2024/17138-0, 2022/12609-9 and 2021/00675-4)

Estudo da influência de nanocristais de celulose na eletrodeposição de Pt sobre eletrodos de grafite/Ti.

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Palavras Chave:*Pt, eletrodos de grafite, nanocristais de celulose, voltametria cíclica.*

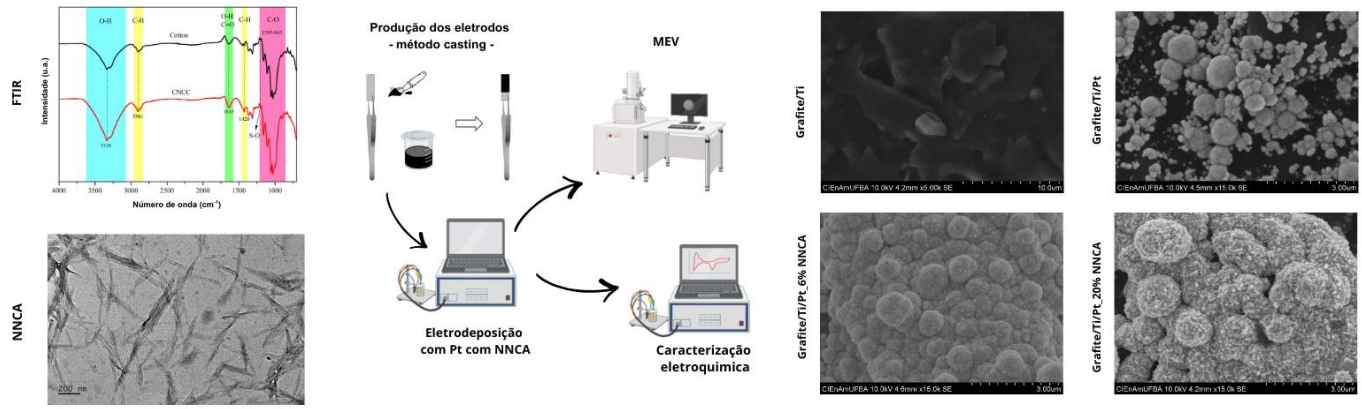
Highlights

Study of the influence of cotton-derived cellulose nanocrystals on platinum electrodeposition on graphite-modified titanium electrodes using cyclic voltammetry.

Resumo/Abstract

Neste trabalho, eletrodos de grafite suportados em titânio, produzidos pelo método*casting,*foram modificados com eletrodepósitos de platina (Pt), na presença ou não de nanocristais de celulose de algodão (NNCA) utilizando voltametria cíclica (VC). Diferentes concentrações de NNCA (0% a 20% (V/V)) foram avaliadas na solução de eletrodeposição. Os diferentes eletrodos obtidos foram caracterizados eletroquimicamente por VC e morfologicamente por MEV. Os NNCA utilizados foram obtidos por hidrólise ácida do algodão. A análise por FTIR destas nanopartículas em comparação ao algodão mostrou bandas de absorção semelhantes, indicando que os NNCA sintetizados se encontram principalmente na forma de celulose e não se observou destruição da estrutura das nanopartículas na extração (1). A caracterização morfológica por MET dos NNCA mostrou uma morfologia em forma de bastonete (1). Sobre o comportamento eletroquímico dos eletrodos obtidos constatou-se que a eletrodeposição da Pt ocorreu sobre os eletrodos estudados e apresenta um perfil de resposta eletroquímica típica de Pt policristalina em soluções ácidas (2). A área eletroquimicamente ativa da Pt foi estimada observando-se um aumento de 4% e 22% para os eletrodos modificados na presença de 6% e 20% NNCA na solução de eletrodeposição, respectivamente. Sobre as caracterizações morfológicas, foi possível visualizar eletrodepósitos de Pt com morfologias diferentes a depender da %NNCA presentes na solução. Em concentrações baixas de NNCA observou-se uma morfologia do tipo globular e para concentrações altas observou-se uma morfologia do tipo de multicasulos (3,4). Os resultados apresentados são ainda preliminares e outras análises estão sendo realizadas para elucidar a participação dos NNCA no processo.

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Procedimento experimental de modificação dos eletrodos, juntamentemente com algumas caracterizações.

Estudo eletrocatalítico de Nb2O5/Al2O3 aplicado à fotoeletrólise da água

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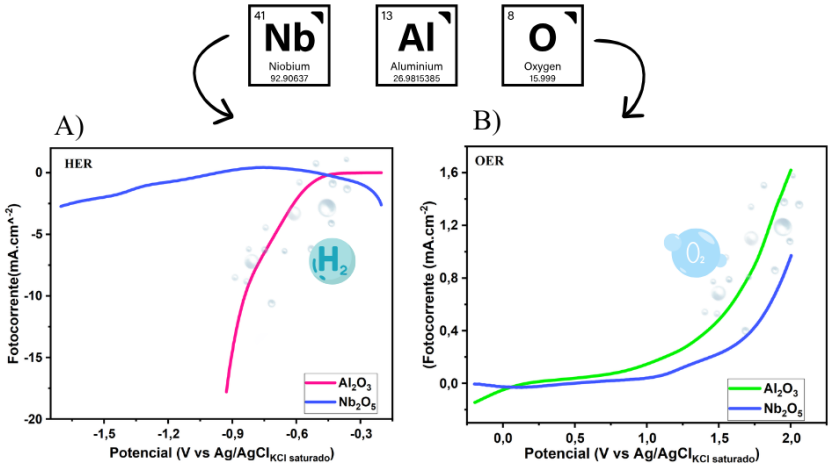
Palavras Chave:*Pentóxido de Nióbio, Óxidos mistos, Fotoeletrodos, Eletrocatálise, Produção de Hidrogênio,Pentóxido de Nióbio, Óxidos mistos, Fotoeletrodos, Eletrocatálise, Produção de Hidrogênio*

Highlights

Nb_2O_5/Al_2O_3 impulsiona a fotoeletrólise da água.
A composição 95:15 eleva a fotocorrente e favorece a OER.
Já 85:15 ativa a HER.
Sistema promissor para H_2 sustentável.

Resumo/Abstract

A fotoeletrólise da água tem se mostrado um cenário promissor para a produção sustentável de hidrogênio, contribuindo para o desenvolvimento de fontes energéticas limpas. Nesse contexto, o pentóxido de nióbio (Nb2O5) apresenta propriedades e características atrativas, como baixo custo e elevada estabilidade fotoeletroquímica. Este trabalho teve como objetivo investigar o desempenho eletrocatalítico e fotoeletroquímico de óxidos mistos de Nb_2O_5/Al_2O_3, aplicado como material de eletrodo para a fotoeletrólise da água. Os filmes estudados foram obtidos pelo método Pechini, com variação da proporção de Nb de 100 até 85% em relação ao Al, visando à obtenção de sistemas homogêneos e com boa dispersão do óxido ativo, maximizando a camada eletroativa disponível. Por meio de análises eletroquímicas e fotoeletroquímicas, foi possível avaliar o comportamento dos fotoeletrodos sob iluminação UV e no escuro, para comparação de resultados. Nas análises de voltametria de varredura linear, a composição de 95:15 apresentou um aumento significativo na fotocorrente se comparada ao material puro em um mesmo potencial, favorecendo a cinética de evolução de oxigênio (OER). Por outro lado, para a evolução de hidrogênio (HER), a composição de 85:15 foi a única entre as proporções, a apresentar atividade catalítica. Esses resultados indicaram que o sistema Nb_2O_5/Al_2O_3 apresenta comportamento promissor, evidenciando seu potencial para aplicações em processos de fotoeletrólise da água e na produção de hidrogênio.



Voltametrias de varredura linear, nas composições de A) 85:15 e 100:0 e B) 95:05 e 100:0 (Nb:Al).

Agradecimentos/Acknowledgments

O presente trabalho foi realizado com apoio do CNPq, da CAPES (Código de Financiamento 001) e da FAPESP (Processos nº [2017/11986-5] e [2025/17294-4]). Agradecemos às agências de fomento pelo suporte fundamental para o desenvolvimento desta pesquisa.

Evaluate the electrochemical performance of 3D sensors for dopamine determination

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Palavras Chave:*3D printing, Lab-made filaments, 3D electrochemical sensors, Dopamine,3D printing,Lab-made filaments,3D electrochemical sensors,Dopamine*

Highlights

Determination of dopamine using a 3D-printed electrochemical sensor.

Resumo/Abstract

The development of 3D sensors using lab-made filaments has increased significantly over the years. Thus, this work proposes the use of lab-made filaments based on Poly(lactic acid) (PLA) modified with Carbon Black (CB) for the development of a 3D sensor for dopamine determination. The filament was fabricated following a simple methodology using a mixture of acetic acid and dichloroethane (3:1 v/v), resulting in a conductive composite filament, with an electrical conductivity of 59.31 ± 0.41 S m^{-1}, this conductivity was calculated by measuring the resistance, in triplicate, of a 2 cm segment of the filament using a multimeter (Figure 1A).This filament was evaluated to develop the 3D electrochemical sensor for Dopamine (DA). Cyclic voltammetry was used to evaluate the voltammetric profile of DA, with the anodic peak observed at 428 mV. With the anodic peak potential defined, a potential range was proposed to be applied in the Differential Pulse Voltammetry (DPV) technique (0.2 to 0.6 V) for DA analysis. We were evaluated and optimized the parameters of the technique DPV (amplitude of 0.125 V and scan rate of 10 mV s^{-1}) and of the reactional environment (phosphate buffer at pH 6.00 and a concentration of 0.2 mol L^{-1}). Under these conditions, an analytical curve was constructed, showing two linear response rangesfrom 0.5 a 4.0 µmol L^{-1} and 5.0 a 30.0 µmol L^{-1}, with a LOD of 0.29 µmol L^{-1} and a LOQ of 0.98 µmol L^{-1} (Figure 1B and C). Furthermore, the devices proved to be reproducible, with a standard deviation of ± 5% in current. Therefore, this sensor proved to be an effective alternative to commercial filaments, as well as being promising for DA determination in real samples.

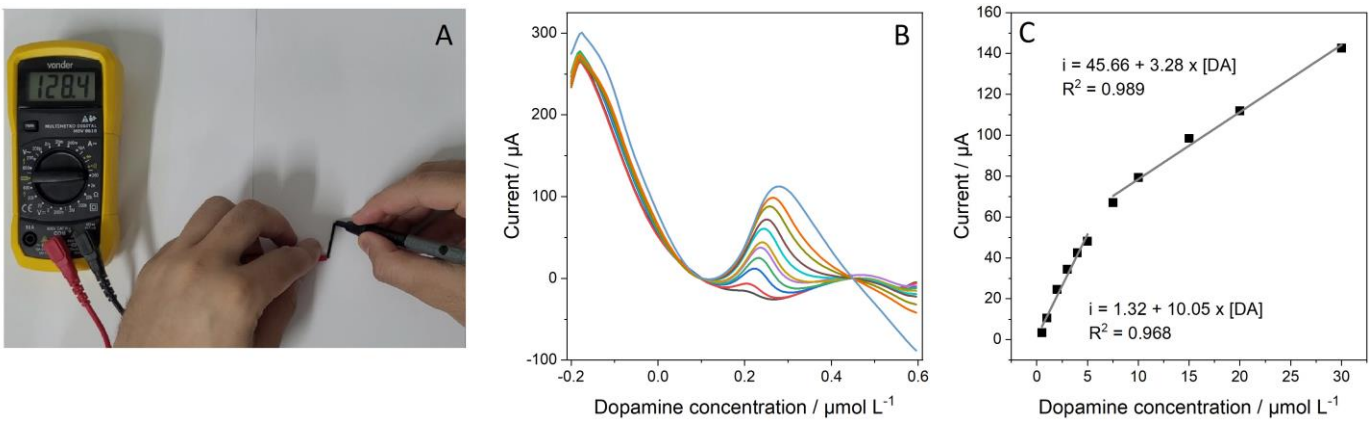


Figure 1. A) Resistance measurement. B) DPV for DA additions. C) Analytical curve.

Agradecimentos/Acknowledgments

UFSJ; DCNAT; FQMAT; INCT-CEMAR; CNPq; CAPES and FAPEMIG.

Evaluation of cycling performance of lithium–sulfur cells assembled with graphene-based functional membranes

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Palavras Chave:*graphene oxide/carbon nanotube composites,functional membranes,lithium–sulfur batteries,cyclability*

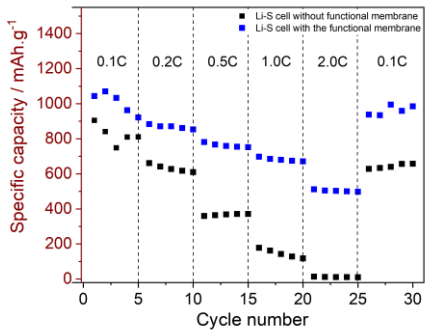
Highlights

Functional graphene oxide/multiwalled carbon nanotube composite membranes were developed for lithium–sulfur batteries.

GO/MWCNT membranes reduce polysulfide shuttling, improving cycling stability.

Resumo/Abstract

Lithium–sulfur (Li–S) batteries offer high theoretical energy density but suffer by high volume variation, insulating nature of sulfur and the polysulfide shuttle, which causes capacity fading. Functional membranes based on graphene oxide (GO) and carbon nanotubes (CNTs) have been explored as interlayers between the cathode and the Celgard separator to mitigate many of these issues. Owing to their conductivity, high surface area, and controllable surface chemistry, GO/CNT membranes act as physical and chemical barriers, reducing polysulfide migration through size exclusion and adsorption. Considering this, in the present work, the electrochemical performance of Li–S cells employing GO/MWCNT functional membranes was evaluated over 500 charge/discharge cycles. The membranes were produced from aqueous suspensions of GO and MWCNT with vacuum-filtration using a Millipore system. The developed membranes were characterized by Raman spectroscopy, thermogravimetric analysis, and scanning electron microscopy. Li–S cells were assembled using a mesoporous carbon/sulfur composite based cathode, metallic lithium anode, Celgard separator, and organic electrolyte, with the GO/MWCNT membrane inserted between the cathode and separator. Electrochemical characterization was accomplished by cyclic voltammetry, electrochemical impedance spectroscopy (EIS), and galvanostatic charge/discharge tests. Cells incorporating the functional membrane delivered higher capacities at all tested C-rates (0.1C–2C) compared to cells without the membrane (see Fig. 1). The cell with the functional membrane showed capacities (at 0.5C) of 746 mAh/g (1st cycle), 524 mAh/g (cycle 250), and 190 mAh/g (cycle 500), higher than those observed for the cell without the functional membrane of 458 mAh/g (cycle 1), 352 mAh/g (cycle 250), and 37 mAh/g (cycle 500) demonstrating the effectiveness of this strategy for improving long-term Li–S battery performance.



Specific capacity at different C-rates for Li-S cells built with/without the functional membrane.

Agradecimentos/Acknowledgments

CNPq (408760/2022-2) CAPES, FAPEMIG, MOVER/FUNDEP, INCT Nanocarbono e Centro de Microscopia da UFMG.

EVALUATION OF SOLAR RADIATION IN THE STUDY OF THE DEGRADATION OF EMERGING CONTAMINANTS AND IN THE PRODUCTIONOF HYDROGEN

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Palavras Chave:*Degradation,Emerging contaminats,Production of hydrogen,Solar radiation*

Highlights

From sunlight to sustainability: photovoltaic systems harness solar energy to degrade pollutants and produce clean green hydrogen.

Resumo/Abstract

The growing demand for clean energy sources and sustainable technologies has intensified interest in solar radiation as a renewable power supply for environmental and energy applications. This study evaluates solar radiation as an energy source for photovoltaic panels and their application in electrochemical processes aimed at the degradation of emerging contaminants and the production of green hydrogen. The proposed system uses solar-powered photovoltaic energy to supply electricity to electrochemical reactors, enabling the oxidation of environmentally relevant pollutants that are often resistant to conventional treatment methods, while simultaneously generating hydrogen through water electrolysis. The photovoltaic panel performance is assessed as a function of solar irradiance, as well as its efficiency in providing stable electrical current to the system. The expected results indicate that integrating solar energy with electrochemical technologies represents a promising strategy for environmental remediation and sustainable hydrogen production. This approach contributes to the development of clean technologies aligned with the principles of green economy and global energy transition.

Agradecimentos/Acknowledgments

The authors thank CNPq for the financial support provided.

Evaluation of the Potential of Macaúba (Acrocomia aculeata) Biochar for Electrochemical Sensors

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Palavras Chave:*Biochar, electrochemical sensors, electroanalysis, electrodes, cyclic voltammetry.*

Highlights

Carbonaceous material derived from lignocellulosic residues enables new pathways for innovation in electroanalysis.

Resumo/Abstract

Electrochemical sensors stand out for their high selectivity, rapid response, and low cost, and are widely used in quality control, clinical diagnostics, and environmental monitoring. In this context, incorporating sustainable materials such as biochar emerges as a promising approach to reconcile analytical performance with environmental responsibility. This study evaluated the effect of adding biochar, obtained from lignocellulosic residues of*Acrocomia aculeata*, a palm native to Brazil belonging to the family Arecaceae and also known as Macaúba, on the electrochemical response of carbon paste electrodes. Three formulations were prepared with 10% (w/w) mineral oil and 90% (w/w) solid phase (graphite + biochar): 90/0, 70/20, and 45/45 (w/w) graphite/biochar. The devices were evaluated by cyclic voltammetry in a 5 mmol L^{-1} ferri/ferrocyanide solution in 0.1 mol L^{-1} KCl. All formulations showed well-defined electrochemical responses. The electrode containing 20% biochar exhibited the best performance, with higher peak currents (~300 µA), smaller peak-to-peak separation (ΔEp ≈ 0.20 V), and an Ipa/Ipc ratio close to unity, indicating more efficient charge transfer and quasi-reversible behavior. The 45% biochar formulation showed an intermediate response (~140 µA, ΔEp ≈ 0.26 V), whereas the biochar-free electrode showed lower electrochemical activity (~100 µA, ΔEp ≈ 0.29 V). The results indicate that controlled biochar incorporation significantly improves electrochemical activity, reinforcing its potential as a sustainable additive in electroanalytical sensors. Future studies should focus on optimizing the composition and on surface functionalization strategies to improve selectivity and analytical sensitivity.

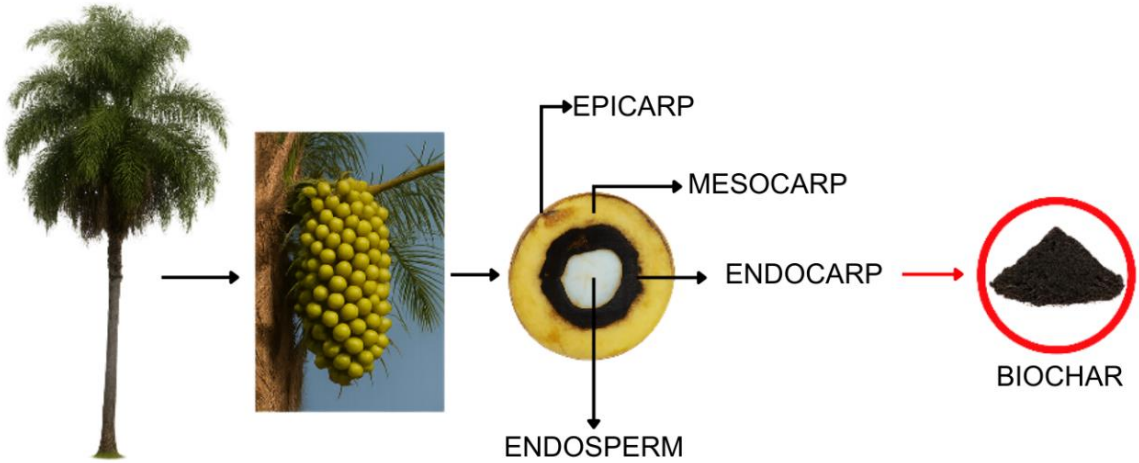


Figure 1: Biochar produced from Macaúba. Source: Prepared by the author using BioRender (2025).

Agradecimentos/Acknowledgments

The authors thank CAPES for the research scholarship and acknowledge CNPq (406419/2021-3 and 408001/2023-2) and FAPERJ (E-26/290.009/2023) for technical and financial support.

Exploring the Ir/Nb_2O_5 interface for the oxygen evolution reaction (OER) in acidic media.

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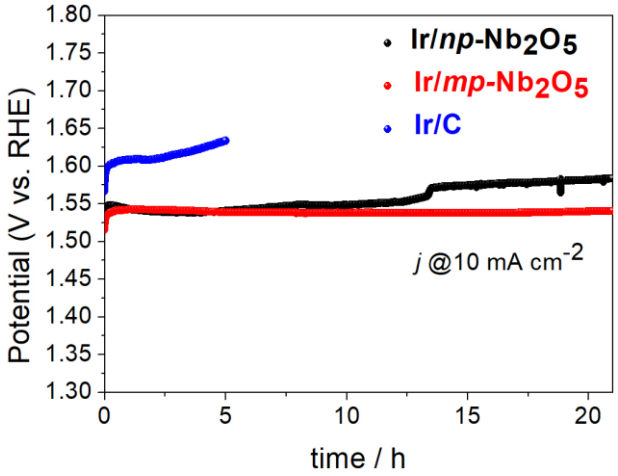
Palavras Chave:*Oxygen evolution reaction,Iridium nanoparticles,Nb2O5 support,Mesoporous oxides*

Highlights

Iridium nanoparticles were supported on Nb_2O_5 nanoparticles and mesoporous Nb_2O_5 architectures. Strong Ir–O–Nb interfacial interactions govern catalytic activity and stability under acidic OER.

Resumo/Abstract

Water electrolysis is a key technology for sustainable hydrogen production, yet its efficiency in proton-exchange membrane (PEM) systems is limited by the sluggish kinetics of the oxygen evolution reaction (OER). Although iridium-based catalysts remain the benchmark for acidic OER, their scarcity and high cost require strategies that maximize activity while minimizing noble-metal loading. Here, we report the synthesis of iridium nanoparticles supported on Nb_2O_5 nanoparticles and mesoporous Nb_2O_5 architectures to investigate the role of Ir–O–Nb interfacial interactions in governing catalytic performance. Structural and chemical characterization was performed using X-ray photoelectron spectroscopy and electron microscopy. Electrochemical measurements in an acid electrolyte (H_2SO_4 0.5 mol L^{-1}) reveal that mesoporous Nb_2O_5-supported Ir exhibits enhanced Ir utilization and a significantly larger electrochemical surface area (886 cm^2) compared to its nanoparticle-supported counterpart (637 cm^2) at 30 wt% Ir loading. While both catalysts display similar OER overpotentials at 10 mA cm^{-2} (275–280 mV), the mesoporous catalyst demonstrates markedly improved durability during prolonged chronopotentiometry experiments, with a potential decay rate of only 0.1 mV h^{-1}, substantially outperforming Ir/np-Nb_2O_5 (2.1 mV h^{-1}) and Ir/carbon (6.6 mV h^{-1}). These results highlight the critical role of mesoporous-structured Nb_2O_5 supports in stabilizing Ir via strong Ir–O–Nb interactions, offering a viable pathway toward durable Ir-efficient OER electrocatalysts for PEM water electrolysis.



Chronopotentiometry curves of the OER catalysts recorded at a constant current density of 10 mA cm^{-2}

Agradecimentos/Acknowledgments

Feasibility Study and Optimization of the Electrochemical Synthesis of Prussian Blue: The Role of pH, K^+, and Chitosan

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Palavras Chave:*prussian blue,mediator,stability,chitosan*

Highlights

Prussian blue with modern biopolymer engineering, paving the way for more stable, efficient, and functional hybrid films for (bio)electrochemical devices.

Resumo/Abstract

This work is based on the modification of electrodes with Prussian blue (PB), a material widely used in the fabrication of sensors and biosensors due to its high sensitivity, stability, and analytical versatility, which includes applications ranging from hydrogen peroxide detection to glucose monitoring – a highly relevant clinical application for diabetes management. Although it exhibits relative stability in aqueous media, PB films show accelerated degradation at neutral and alkaline pH, limiting their use under certain conditions. This study investigated the formation of PB films in the presence and absence of deacetylated chitosan, in buffer solutions at pH 4.5, 6.0, and 7.0 containing different anions (acetate, phosphate, and citrate), with and without the addition of potassium ions (K^+). The results demonstrate that chitosan acts as a stabilizing matrix, promoting a more homogeneous immobilization of PB on the electrode surface and forming a protective layer that preserves its catalytic activity. It was also observed that the presence of K^+ in the electrolyte solution is crucial for film stability, as the redox mechanism of PB involves the insertion and deinsertion of this ion into its cubic structure. This dependence was evident in tests performed in phosphate buffer at pH 6.0, where the absence of K^+ led to rapid film decomposition. In conclusion, the association between PB and chitosan represents a promising strategy for the development of more robust electrochemical biosensors, paving the way for the rational design of modified films with functionalized biopolymers for specific analytical applications.

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FCFRP-USP, INCT Bioanalitica

From Ion Transport to Interface Stability: A Comparative Study of Sodium-Based Electrolytes via Operando FTIR analysis

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Palavras Chave:*sodium-based supercapacitor,electrolyte,ionic liquid,eutectic solvent,operando Fourier-transform infrared spectroscopy*

Highlights

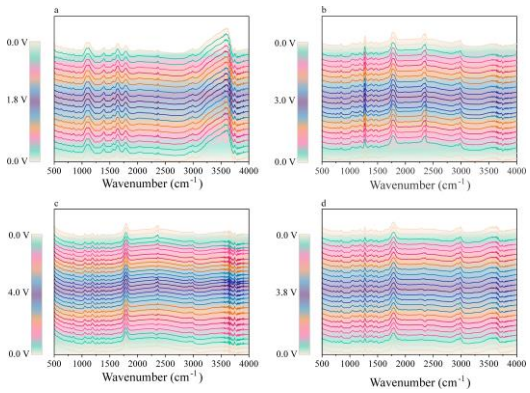
Electrolyte chemistry dictates sodium supercapacitor performance.
Ionic liquids enable high energy density.
Eutectic solvents show balanced stability/mobility.
Operando FTIR tracks interface evolution.

Resumo/Abstract

Electrolyte chemistry plays a central role in the performance and reliability of sodium-based supercapacitors (SCs), as it directly affects ion transport, electrochemical stability, and interfacial reactions. This work presents a comparative assessment of four representative sodium-based electrolyte families: water-in-salt electrolytes, organic carbonate systems, ionic liquids (ILs), and deep eutectic solvents (DESs). Conventional electrochemical techniques, including cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy, are combined with operando Fourier-transform infrared spectroscopy (FTIR) to investigate how electrolyte composition governs charge storage behavior and interface chemistry.

Clear differences are observed across the electrolyte classes. The $NaClO_4$:$[C_3mpip][NTf_2]$ IL exhibits the highest capacitance and energy density, enabled by its wide electrochemical stability window and chemically stable electrode interfaces. The NaOTf:PEG400 DES shows intermediate electrochemical performance, offering a balance between ionic mobility and interfacial robustness, with improved stability compared to aqueous systems. In contrast, the 17 m $NaClO_4$ WiSE electrolyte, despite its high ionic conductivity, displays pronounced interfacial degradation that restricts the accessible voltage range and limits long-term performance.

Operando FTIR measurements reveal electrolyte-dependent interfacial transformations during polarization, highlighting differences in ion coordination, solvent reactivity, and surface species formation. These findings demonstrate that high ionic conductivity alone does not guarantee superior electrochemical performance, and that interface stability is a decisive factor.
Overall, this comparative study establishes clear relationships between electrolyte chemistry, interfacial evolution, and electrochemical response, providing practical guidelines for the selection and design of electrolytes for sodium-based SCs.



Operando FTIR spectra during polarization reveals electrolyte-dependent interfacial evolution.

Agradecimentos/Acknowledgments

We are grateful for the financial support from Shell, the strategic support from ANP (Brazil's National Oil, Natural Gas, and Biofuels Agency) and the Brazilian funding agency CAPES, and the assistance of OpenAI ChatGPT-5 for grammar refinement.

Gold Modification Strategies for 3D-Printed Electrodes: Drop-Casting vs Electrodeposition Effects on Electroactive Surface Area

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Palavras Chave:*Additive manufacturing,Electrochemistry devices,AuNPs,Dopamine,Detection*

Highlights

Surface electrodes were activated by AirPlasma pen; AuNPs pre-synthesized improved electroactive surface of 3D printed electrodes.

Resumo/Abstract

In recent years, 3D-printed electrodes have emerged as promising platforms for electrochemical applications, with surface functionalization being a key factor determining their performance. In this context, this work aims to investigate the differences between modifying the electroactive surface with pre-synthesized gold nanoparticles (AuNPs) and gold electrodeposition. Electrodes measuring 6.0 x 26 x 1.6 mm were printed using a commercial conductive filament based on PLA and carbon black (Protopasta®). The working surfaces were activated by air plasma using a Plasmax® pen at 3 W in continuous discharge mode, applied with a 0.20 × 15 mm needle. For surface modification, 20 µL of AuNPs ($3x10^{17}$ NP mL^{-1}) were drop-cast onto selected electrodes, while others were modified by gold electrodeposition via chronopotentiometry at a potential of 0.5 V for 40 seconds. The electrodes were characterized by cyclic voltammetry (CV) using a 5:5 mmol L^{-1} $[Fe(CN)6]^{3-/4-}$ solution in 0.1 mol L^{-1} KCl, followed by dopamine (DA) detection. CV results showed that the electrode modified with AuNPs droplet deposition exhibited a DA oxidation peak of 2.4 µA at 75 mV s^{-1}, whereas the electrode modified by electrodeposition exhibited a lower signal of 1.1 µA. Overall, electrodes modified with AuNP drop-casting exhibited enhanced electrochemical responses compared to electrodeposition. This may be correlated with differences in surface structure:pre-synthesized AuNPs possess high-energy crystallographic planes, while electrodeposition likely produces a more uniform and stable gold film, which may reduce catalytic activity on the electrode surface. The results obtained so far are promising and suggest that functionalization of 3D-printed electrodes with pre-synthesized AuNPs can overcome detection limitations. Further investigations will be conducted to better understand these systems and evaluate their performance in detecting analytes such as DA.

Agradecimentos/Acknowledgments

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Influência de materiais carbonáceos no comportamento eletroquímico de eletrólitos de vanádio para baterias de fluxo redox.

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Palavras Chave:*Materiais Carbonáceos,Voltametria Cíclica,Baterias de Fluxo Redox,Carbono Vítreo,Eletrólitos*

Highlights

The influence of carbon-based materials on the electrochemical behavior of vanadium electrolytes for redox flow batteries. Carbon increases current density.Three-electrode cell.

Resumo/Abstract

A busca por alternativas sustentáveis para armazenamento de energia tem impulsionado o desenvolvimento de baterias de fluxo redox (RFB), nas quais a energia é armazenada em espécies redox dissolvidas em eletrólitos líquidos que circulam por uma célula eletroquímica. Neste trabalho, avaliou-se a influência de carbono condutor nas propriedades eletroquímicas do eletrólito de vanádio.

Para tanto, preparou-se uma solução de vanádio 1,4 mol/L, da qual foram separadas alíquotas contendo 0,1% m/m de carbono condutor. Em seguida, as amostras foram analisadas por voltametria cíclica (VC) utilizando três eletrodos: carbono vítreo (trabalho), platina (contra-eletrodo) e Ag/AgCl (3 mol/L) (referência). As medidas foram realizadas com janela de potencial E = (-0,1 V; 1,6 V; -1,0 V), velocidade de varredura de 50mV/s e 3 ciclos. A Fig. apresenta dois voltamogramas: em vermelho, o resultado sem carbono condutor e, em azul, na presença desse composto. Ambos apresentam aumento de corrente positiva entre 1,0-1,4 V e negativa entre 0,7-0,1 V. Esse aumento de corrente está relacionado com a oxidação e redução do par redox V 4+ /V 5+ . Ainda, nota-se aumento de corrente e deslocamento de potencial na presença de carbono condutor, evidenciando que materiais carbonáceos facilitam a transferência eletrônica e indicam maior reversibilidade do sistema. O eletrólito de vanádio é composto por uma mistura equimolar de V 4+ /V 3+ e era esperada a visualização de um processo em potenciais mais negativos relacionados com o V 3+ /V 2+ . Provavelmente, essa supressão de sinal está relacionada com o material do eletrodo utilizado. Futuramente, pretende-se repetir os experimentos com feltro de carbono e outros materiais carbonáceos, como grafite e grafeno. Em conclusão, a adição de carbono condutor aumentou significativamente a corrente do eletrólito, indicando melhor transferência de carga e maior reversibilidade do sistema.

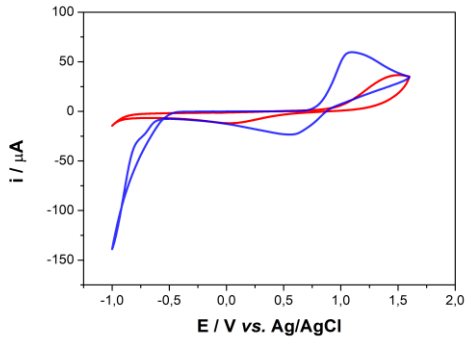


Fig.VC do eletrólito de vanádio (1,4 mol/L) sem (vermelho) e com carbono condutor(azul). v=50mV/s.

Agradecimentos/Acknowledgments

Agradecemos ao CNPq pelo apoio financeiro e pela concessão de auxílio à pesquisa(Processo nº 446787/2024-8, 314945/2025-3,192395/2025-4).

INFLUÊNCIA DOS TRATAMENTOS FÍSICO, QUÍMICO E ELETROQUÍMICO NOS ELETRODOS 3D

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Palavras Chave:*Voltametria; Tratamento eletroquímico; Monitoramento ambiental*

Highlights

3D-printed electrodes enhance voltammetric detection of sulfamethoxazole.

Treated electrodes show higher current density for sulfamethoxazole detection

Resumo/Abstract

O sulfametoxazol (SMX) é um antibiótico utilizado para tratar infecções bacterianas, que é parcialmente excretado na forma original [1] e apresenta resistência a processos convencionais de tratamento de efluentes, sendo detectado em matrizes aquáticas com concentrações que podem oferecer riscos ambientais. Com isso, este estudo avalia o desempenho de eletrodos impressos em 3D (E3D), produzido a partir de um filamento de ácido polilático contendo*carbon black,*na determinação voltamétrica do SMX bem como a influência de tratamentos físico, químico e eletroquímico sobre sua resposta analítica. Para isso, foi utilizado um sistema eletroquímico convencional de três eletrodos, com o E3D sendo o de trabalho, o Ag|AgCl|$KCl_{(sat.)}$ como eletrodo de referência e platina como contraeletrodo. Os tratamentos foram realizados de forma individual (apenas um tratamento realizado no eletrodo) e também de maneira sequencial (os três tratamentos aplicados sucessivamente a um mesmo eletrodo). O tratamento físico consiste em polimento da superfície; o químico na imersão em solução de hidróxido de sódio 0,5 mol L^{-1} sob ultrassom por 30 min; e o eletroquímico na aplicação de potenciais de +1,4 e −1,0 V[2].As medidas foram realizadas por voltametria cíclica em uma faixa de 0,0 a +1,8 V; com uma velocidade de varredura de 0,05 V s^{-1}, usando como eletrólito suporte ácido sulfúrico 0,5 mol L^{-1}. Os resultados obtidos demonstraram que o tratamento sequencial promoveu um aumento de 31% na densidade de corrente de em relação ao eletrodo submetido apenas ao tratamento físico, obtendo um potencial de oxidação definido em 1,23 V. Isso evidencia que a combinação dos processos otimiza a eficiência do E3D na detecção do medicamento.

Ref**.**

[1] Yeh, S.-H.; Huang, M.-S.; Huang, C.-H.*J. Taiwan Inst. Chem. Eng.*,**131**, 104155 (2022).

[2] Rodrigues, J. G. A.*et al.ACS Omega*,**10**, 1131–1143 (2025).

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Influence of Au/WO3 heterojunctions and plasmonic excitation on electrochemical and optical properties for green hydrogen production.

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Palavras Chave:*Plasmonics,WO3,Gold nanoparticles,Photoelectrochemistry,Green hydrogen*

Highlights

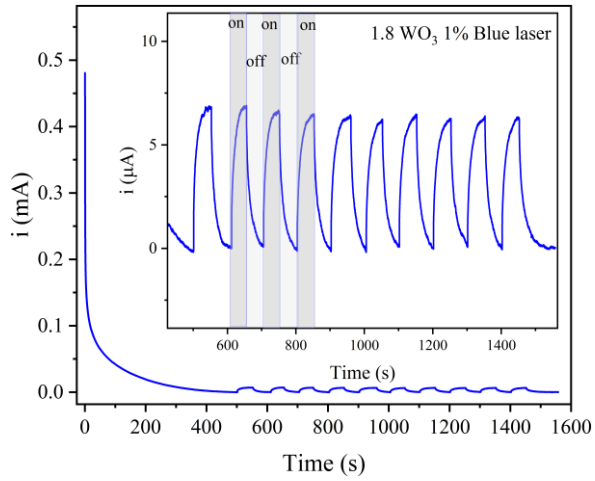
Au/WO_3 heterojunctions modulate charge transfer under plasmonic excitation. Blue light enhances electrochemical activity via hot charge carriers. Au loading strongly affects electrochemical behavior.

Resumo/Abstract

The electrochemical production of green hydrogen is a promising strategy for energy storage from renewable sources. However, it is still limited by kinetic barriers associated with the oxygen evolution reaction. In this context, plasmon-assisted electrochemistry emerges as an alternative to reduce overpotentials and enhance charge-transfer processes. In this work, the influence of Au/WO_{3-x} heterojunction on plasmonic excitation on the electrochemical and optical properties of the materials was investigated.

WO_{3-x} based catalysts containing different Au loadings (1, 2, and 5 wt%) were obtained through mechanochemical processing. Glassy carbon electrodes were modified by drop casting the catalyst and used as working electrodes. The measurements were done in acidic medium (0.5 mol L^{-1} H_2SO_4) using a three-electrode electrochemical cell. Cyclic voltammetry and spectroelectrochemical experiments in the UV-Vis were performed in the dark and under laser irradiation at different wavelengths, including chopped illumination conditions.

The results showed that the Au loading plays a decisive role in the electrochemical behavior of the materials. The system containing 1 wt% Au exhibited better nanoparticle dispersion, favoring charge transfer and resulting in greater electrochemical stability. In contrast, higher Au contents led to irregular electrochemical and optical responses, attributed to Au nanoparticle agglomeration. Under blue laser irradiation, an increase in current density and the emergence of additional redox processes were observed, evidencing the participation of hot charge carriers generated by localized surface plasmon resonance. Spectroscopic analyses indicated variations in the band gap as a function of the applied potential and the wavelength of the incident light, reinforcing the strong correlation between electronic structure, plasmonic optical excitation, and electrochemical activity.



Chronoamperometric response of WO_3–1% Au NPs under blue laser on–off illumination.

Agradecimentos/Acknowledgments

FAPESP: #2022/06405-1; #2024/02870-7; #2025/12347-2

Influence of keratin extracted from chicken feathers on activated carbon derived from peach pits for application in energy storage devices.

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Palavras Chave:*Peach pits, chicken feathers, keratin, activated carbons, supercapacitors.*

Highlights

Activated carbons from peach pits and chicken-feather keratin enable circular-economy electrodes with specific capacitance up to ~124 F g^{-1} (3-electrodes system) in 1 mol L^{-1} H_2SO_4.

Resumo/Abstract

According to the United Nations Global Compact and the Sustainable Development Goals (SDGs), the transition to renewable energy (RE) sources and the responsible use of resources are global priorities. However, due to the intermittency of RE, demands efficient energy storage devices such as supercapacitors (SCs), whose performance strongly depends on the electrode materials. In this context, low-cost activated carbons derived from biomass waste and modified with heteroatom-rich dopants emerge as a promising strategy to enhance electrochemical performance while promoting circular-economy principles.

In this work, pulverized peach pits (PD) were used as a biomass precursor and impregnated with keratin (Q) extracted from white chicken feathers. Chemical activation was carried out using 25 % H_3PO_4 with a biomass:activating agent ratio of 1:4. A precursor mixture containing 90 wt% PD and 10 wt% Q (PDQ) was prepared, and activated carbons were synthesized via two routes: direct impregnation and pre-carbonization at 450 °C prior to impregnation. The materials were then pyrolyzed at 700, 800, and 900 °C under N_2 atmosphere. The PD, Q, and PDQ precursors were characterized by Fourier transform infrared spectroscopy (FTIR) to identify functional groups and by thermogravimetric analysis (TGA) to evaluate their thermal decomposition. Textural properties analyzed by N_2 and CO_2adsorption show surface areas up to ~ 948 m^2 g^{-1} (BET) and high microporosity (~ 874 m^2 g^{-1}) for samples at 800 °C using Method 2. Electrochemical evaluation by cyclic voltammetry in 1 mol L^{-1} H_2SO_4 (**Figure 1a)**shows that peach pits activated carbons ($CAD1_{800}$ and $CAD2_{800}$) and their keratin-modified 10 wt % Q ($CAH1_{800}$and $CAH2_{800}$) exhibit a quasi-rectangular profile and enhanced capacitance upon keratin modification, reaching ~124 F g^{-1}. These results highlight keratin as an effective dopant to enhance the electrochemical performance of biomass-derived activated carbons for supercapacitor electrodes.

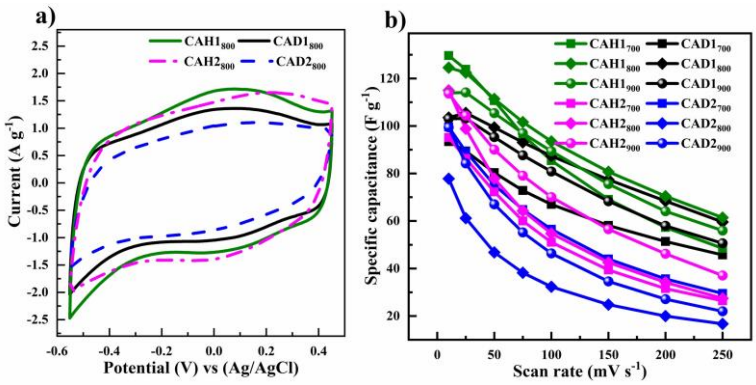


Fig.1. a) CV of AC at 800 °C (10 mV s-1) and b) Cs for AC materials at 700-900 °C (10-250 mV s-1)

Agradecimentos/Acknowledgments

This work was funded by CONCYTEC and PROCIENCIA within the framework of the E077-2023-01-BM Competitions 'Scholarships in Doctoral Programs in Interinstitutional Alliances' N.º PE501084300-2023-PROCIENCIA-BM.

Inibição da corrosão do aço carbono 1020: potencial do óleo de Annona muricata L.

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Palavras Chave:*Óleo de graviola,Adsorção,Perda de massa*

Highlights

Óleo de Graviola demonstra elevado potencial como inibidor sustentável da corrosão do aço carbono 1020 em ambientes agressivos.

Resumo/Abstract

A corrosão consiste em um processo químico espontâneo que ocasiona prejuízos em múltiplos ambientes. Estima-se perdas anuais de 4% do Produto Interno Bruto (PIB) global. No Brasil, em 2023, os custos chegaram a R$ 368 bilhões[1].No presente trabalho, avaliou-se a corrosão do aço carbono 1020 em soluções NaCl 3,5% e HCl (0,1M), bem como a eficiência do óleo de Annona muricata L (óleo de graviola) como inibidor de corrosão. Ensaios gravimétricos foram conduzidos na ausência e presença do inibidor nas concentrações de 0,5 e 1,0% (v/v), em solução salina por 2 h e em meio ácido por 24 h, analisando-se a influência do meio e concentração do inibidor. Em solução salina, na ausência de inibidor, observou-se perda de massa progressiva e aproximadamente linear, característica de corrosão generalizada, induzida por íons Cl^-. A adição do inibidor promoveu redução da perda de massa, com eficiência moderada em relação ao aumento da concentração, sugerindo adsorção superficial e tendência à saturação. Já em meio ácido, na ausência do inibidor, a corrosão mostrou-se mais severa. Contudo, a presença do inibidor resultou significativa redução da corrosão, alcançando eficiência de inibição superior a 80% na concentração de 1,0% (v/v). Ressalta-se que a comparação entre os meios é de caráter qualitativo, uma vez que os ensaios foram realizados em tempos distintos. No entanto, os resultados evidenciam o potencial do óleo de graviola como inibidor de corrosão natural, sustentável e de baixo impacto ambiental para a proteção do aço carbono 1020 em diferentes condições corrosivas.

[1]FERREIRA, H. V. S.; CARVALHO, A. L. C. C.; VIEIRA, R. A. L.; Autor, A.A.; Autor, B.B.; Casos de corrosão e degradação em monumentos históricos de São Luís.**Revista contemporânea**, v. 3, n 12, 2023. Publicado em 2023-12-01. DOI: https://doi.org/10.56083/RCV3N12-251.

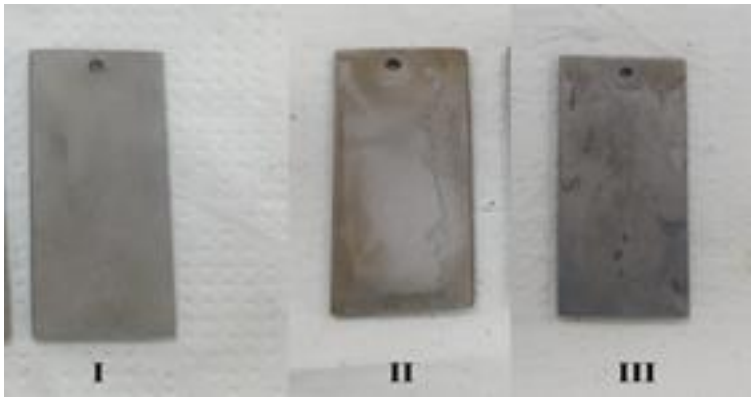


Figura 1: Corpo de prova pós imersão no meio ácido, sem (I) e com inibidor a 0,5 % (II) e 1,0% (II).

Agradecimentos/Acknowledgments

Agradecemos à FAPERJ, ao CNPq e à CAPES.

Investigação do comportamento eletroquímico do óxido de nióbio em eletrodos modificados com filmes compósitos a base de quitosana

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Palavras Chave:*Eletroquímica,semicondutor,interfaces*

Highlights

Filmes compósitos poliméricos a base de quitosana evidenciam eletroatividade do óxido de nióbio.

Resumo/Abstract

Devido à sua estabilidade química, baixa toxicidade e propriedades de superfície, os óxidos de nióbio vem sendo cada vez mais explorados na eletroquímica, por exemplo, em dispositivos como biossensores[1]. Neste trabalho, eletrodos impressos comerciais de carbono, da marca DropSens, modelo DRP 150, foram modificados com filmes compósitos à base de quitosana (QT), grafite (C) e óxido de nióbio e caracterizados por voltametria cíclica, no bipotenciosato portátil DropSens µSTAT400. Os ensaios foram realizados na janela de potencial de −0,2 a 0,6 V, em solução de $K_4[Fe(CN)_6]/K_3[Fe(CN)_6$ (0,01M) em KCl (0,50M), nas velocidades de varredura 10, 20, 50 e 100 mV s^{-1}, após 10 ciclos de estabilização. Os resultados obtidos evidenciaram que os eletrodos contendo apenas quitosana e óxido de nióbio apresentaram resposta faradaica mensurável, caracterizada por pico anódico isolado, o que indica atividade eletroquímica do óxido de nióbio mesmo na ausência de uma fase condutora adicional. No entanto, a ausência do pico catódico e os baixos valores de corrente demonstram limitação na condução eletrônica. Com a introdução do grafite no compósito, observou-se aumento expressivo na corrente e definição dos picos anódico e catódico do sistema, evidenciando a necessidade de uma fase condutora adicional para melhoria da cinética eletroquímica. A comparação com os eletrodos não modificados reforça o caráter semicondutor desses materiais. Portanto, o óxido de nióbio se mostrou eletroquimicamente ativo em sistemas modificados com filmes compósitos a base de quitosana e grafite, na janela de potencial estudada, apresentando reprodutibilidade e indicando que a presença de uma fase condutora adicional melhora seu desempenho eletroquímico. Esse estudo contribui para investigação da influência de óxidos de nióbio em estudos de eletroquímica de interfaces.

[1]GOTARDI, Jessica*et al*. Electrochemical Biosensors Based on Niobium-containing Oxides: A Review.**Analytica Chimica Acta**, p. 344239, 2025.

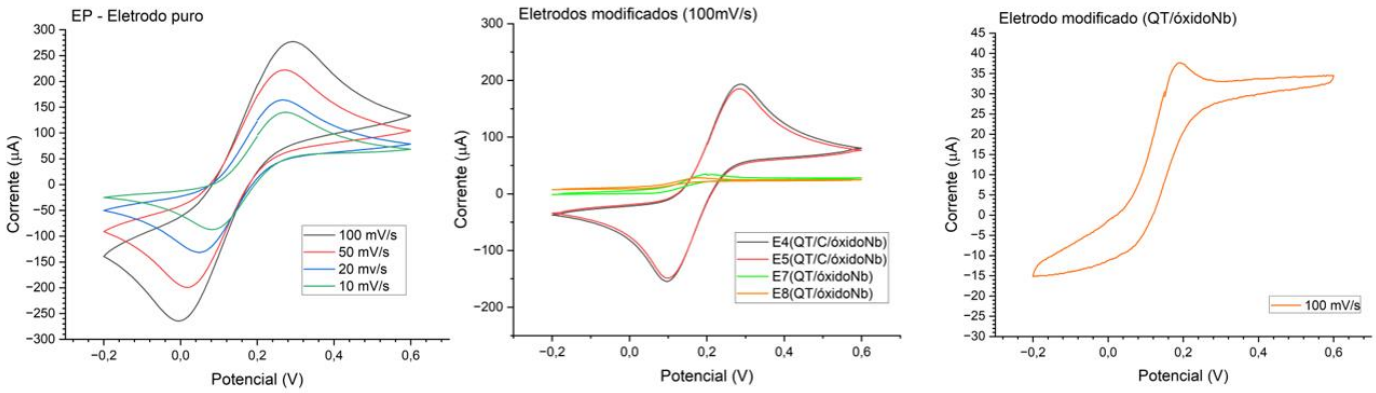


Figura 1: Voltamogramas dos eletrodos puros e modificados com QT/C/óxido de nióbio.

Agradecimentos/Acknowledgments

Agradecemos à FAPERJ, ao CNPq e à CAPES.

Investigation of Triclinic and Hexagonal Birnessite as Water Oxidation Catalysts: A Theoretical and Experimental Study

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Palavras Chave:*water oxidation,electrocatalysis,minerals*

Highlights

This research investigates birnessite based manganese oxides as low-cost OER electrocatalysts for sustainable hydrogen production, focusing on the transformation between triclinic and hexagonal form.

Resumo/Abstract

This work investigates birnessite, a manganese oxide mineral, as a low-cost catalyst for the oxygen evolution reaction (OER) toward low-emission hydrogen production. Birnessite commonly occurs in two phases, triclinic and hexagonal, which can coexist, although only the hexagonal phase is active for OER. Accordingly, both phases were synthesized and comprehensively characterized by SEM, Raman spectroscopy, XRD, XPS, TGA, DSC, and electrochemical measurements. In addition, phase interconversion pathways (between the two birnessite phases and/or toward other Mn-oxide phases) were examined as a function of pH, temperature, and applied potential. Finally, density functional theory (DFT) calculations using VASP were performed to elucidate the OER reaction mechanism in alkaline media on hexagonal birnessite.

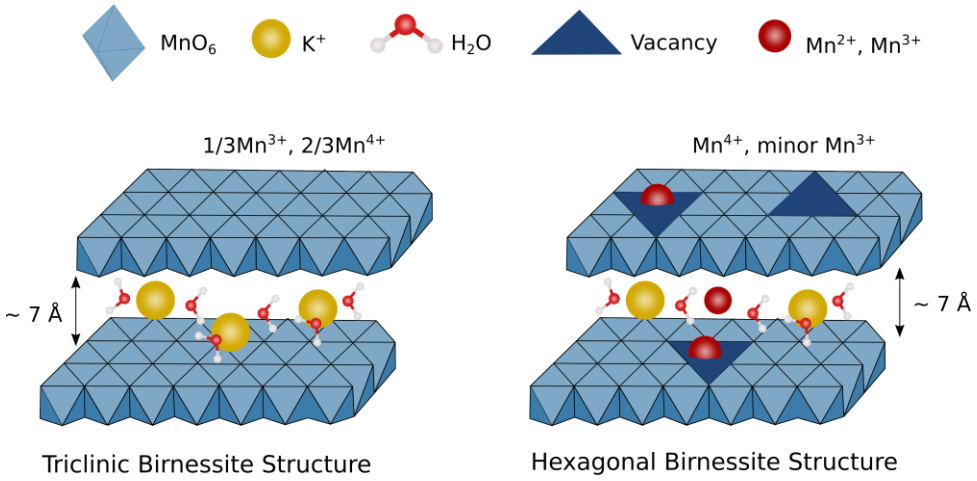


Illustration of birnessite in the triclinic and hexagonal phases.

Agradecimentos/Acknowledgments

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FAPESP-2017/11986-5, 2021/05976, 2024/09666-6.

In vitro electrochemical study of DGTF nitrocompounds: mechanistic implications and reductive bioactivation

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Palavras Chave:*Nitroaromáticos; Voltametria; Mecanismo EC; Bioativação redox; Química medicinal*

Highlights

DGTF nitrocompounds show multistep electrochemical reduction. First reduction forms a stable nitro radical anion. Data support reductive bioactivation relevant to drug design.

Resumo/Abstract

O aumento das doenças infecciosas, especialmente as tropicais negligenciadas, contrasta com a escassez de fármacos eficazes, seguros e acessíveis [1]. Nesse cenário, a busca por novos candidatos, como compostos nitroaromáticos, tem se intensificado [2], destacando a bioeletroquímica como ferramenta estratégica no planejamento molecular e na elucidação de mecanismos de ação [3]. O presente estudo investigou o comportamento eletroquímico*in vitro*de nitrocompostos, denominados DGTFs. Voltamogramas cíclicos (VCs) e de pulso diferencial (VPDs) foram obtidos em eletrodo de carbono vítreo, em meio aprótico ($CH_3CN/TBAPF_6$ 0,1 M), visando mimetizar ambientes lipofílicos de matrizes biológicas. O VC (Fig.1A) do nitrocomposto DGTF15 revelou múltiplas ondas catódicas, indicando um mecanismo redox multietapas típico de nitroaromáticos [3,4,5]. As varreduras dos potenciais de inversão demonstraram que apenas a primeira onda catódica é reversível, associada à formação do ânion radical do grupo nitro, eletroquimicamente estável na escala de tempo da técnica, em concordância com estudos clássicos em meio aprótico [4,5]. As etapas subsequentes apresentaram caráter irreversível, atribuídas a reações químicas acopladas, como dimerização ou novas transferências eletrônicas. O VPD (Fig.1B) confirmou a presença de processos redox distintos, com picos bem resolvidos, corroborando a atribuição mecanística. Em conjunto, os dados evidenciam um mecanismo do tipo EC, coerente com a estrutura do DGTF15 e compatível com processos de bioativação redutiva, reforçando o potencial da eletroquímica no planejamento racional de novos candidatos a fármacos nitroaromáticos.**Referências:**[1] PAOLI-LOMBARDO, R. et al.*Pharmaceuticals*, 2022. [2] KANNIGADU, C.; N'DA, D. D.*Curr.Pharm. Des.*, 2020. [3] XAVIER, J. A. et al.*Curr. Opin. Electrochem.*, 2021. [4] HUANG, Y.; LESSARD, J.*Electroanalysis*, 2016.[5] Santos et al., ChemElectroChem, 2025.

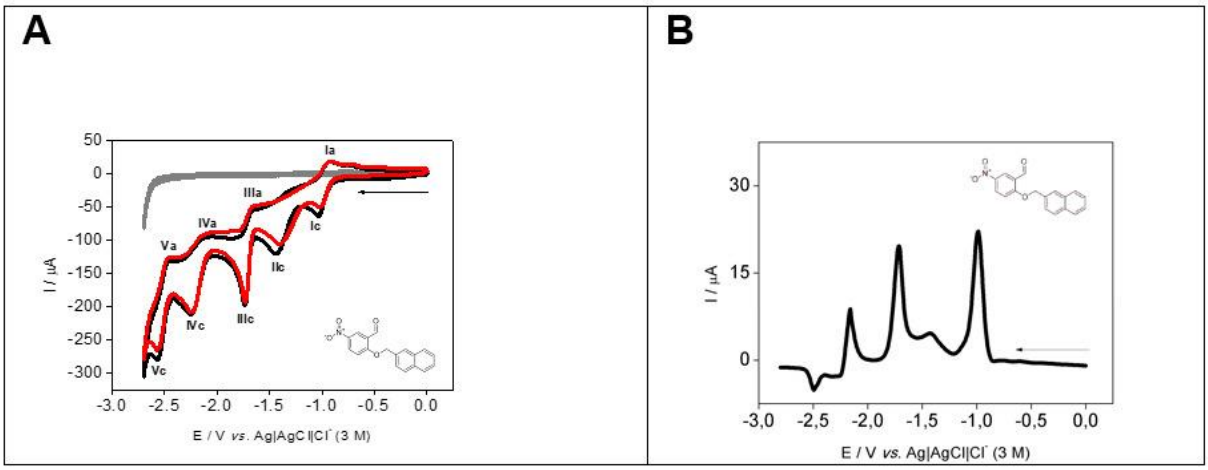


Figura 1. (A) VCs catódicas do composto. (B) VPD da redução do composto.

Agradecimentos/Acknowledgments

FAPEAL, CNPQ, CAPES, RENORBIO, INCTBIO, UFAL and PET Química.

Laser-induced cobalt oxide entrapment within 3D-printed carbon electrodes for amperometric sensing

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Palavras Chave:*3D printing,Laser scribing,Modified electrochemical sensors,Sustainable modification*

Highlights

3D-printed carbon electrodes modified by laser irradiation

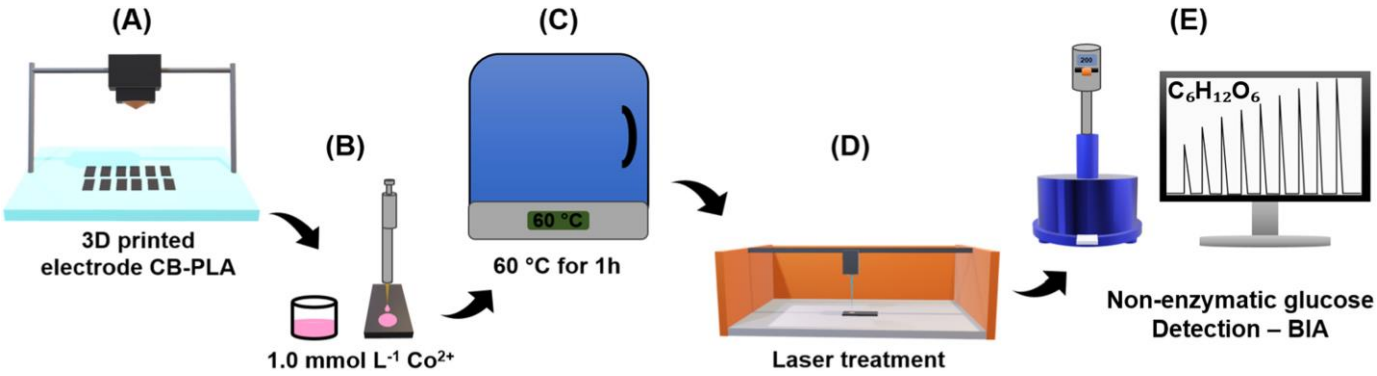
In situ formation of cobalt oxides on the surface

Improved glucose sensing performance

Low-cost and sustainable sensor fabrication

Resumo/Abstract

The 3D printing technology has the ability to manufacture electrochemical sensors in complex three-dimensional shapes with high efficiency and precision. In parallel, laser scribing technology has been employed to manufacture low-cost and disposable electrochemical sensors. Hence, the combination of both technologies can bring numerous possibilities in the field of electrochemical sensors. The present work addresses the possibility of modifying the surface of 3D printed electrodes through a highly sustainable, practical, and inexpensive route using laser irradiation. For this, a surface modification of a carbon black-based 3D printed electrode was performed using a cobalt chloride solution dropped onto the electrode surface, followed by blue laser irradiation. With this, it was possible to provide an improved electrochemical sensor modified in situ with cobalt oxides, as further attested by physicochemical and electrochemical characterizations. The modified sensor was employed for glucose (GLU) determination using a Batch Injection Analysis (BIA) system. From the modification, the cobalt oxides upon the electrode surface allowed the sensitive detection of GLU in a linear range from 50.0 to 400.0 µmol L−1 and LOD of 6.3 µmol L−1. The GLU analysis in the biological samples yielded recovery values close to 100 %, demonstrating good applicability of the sensor. Thus, the combination of 3D printing and laser scribing technology enabled the production of modified sensors that are highly robust and capable of performing the selective detection of GLU in an easy and simple way.



Summary of the production and modification method for the 3D printed electrochemical sensor.

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Mechanism Insights into Plasmon-Assisted N2 and CO2 co-electrolysis on Silver Nanoparticles supported on Heterojunctions

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Palavras Chave:*Silver nanoparticles, Bismuth nanoparticles, Plasmonic catalysis, C-N coupling, N2 reduction reaction*

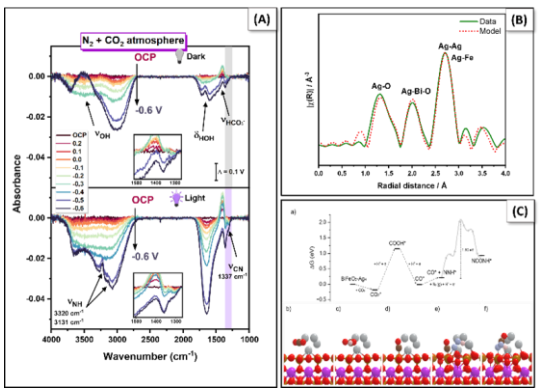
Highlights

One-pot mechanochemical synthesis of NPs over semiconductor heterojunction, Electrocatalysis assisted by Localized Surface Plasmon Resonance (LSPR) of NPs, N_2 and CO_2 co-electrolysis under LSPR

Resumo/Abstract

The N_2 and CO_2 co-electrolysis have attracted attention as an alternative to the energy intensive process for urea synthesis. Here we reported the contribution of localized surface plasmon resonance (LSPR) of Ag NPs supported on heterojunctions, Ag@$BiVO_4$/$BiFeO_3$, during the N_2 + CO_2 co-electrolysis. Our results demonstrated that exciting in the LSPR region of Ag NPs the Faradaic Efficiency and urea yield rate was improved with a reduced overpotential, 24.4% and 19.2 μmol h^{-1} g^{-1} at +0.1 V vs RHE compared to 9.4% and 9.6 μmol h^{-1} g^{-1} at -0.2 V vs RHE under dark conditions. Further*in situ*FTIR-IR investigations, Fig. 1A, demonstrated that under dark and N_2 + CO_2 atmosphere conditions, no huge signals related to nitrogen-intermediates were observed, otherwise a strong adsorption of H_2O over catalyst surface was observed leading to HER. Under LSPR and N_2 + CO_2 conditions, signals related to nitrogen-intermediates were observed at 3320, 3131 and 1337 cm^{-1} related to the urea formation. In relation to H_2O species, an opposite behavior was observed, revealing that under LSPR conditions, H2O species are not easily absorbed over catalyst surface and then HER is suppressed.

As the Ag@$BiVO_4$/$BiFeO_3$, prepared mechanochemically, possesses a complex structure, X-Ray Absorption Spectroscopy (XAS) experiments were carried out, Fig. 1B, to understand its structure and identify the possible catalytic sites involved in the urea electrosynthesis. XAS data showed that in addition to the expected Ag-Ag scattering for Ag species, other domains are present in the catalyst structure, such as Ag-O, Ag-Bi-O and Ag-Fe. Theoretical calculations considering different types of possible structures, revealed that a cluster $BiFeO_3$-Ag_4 plays an important role in the free energy profile for the C-N coupling to give NCONH*, Fig. 1C. In addition, the theoretical calculations agree with XAS data and intermediates observed on*in situ*FTIR-IR experiments.



In situ FTIR-RAS, Ag K-edge EXAFS and free energy profile of NCONH formation on Ag@$BiVO_4$/$BiFeO_3$

Agradecimentos/Acknowledgments

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NEW PETG/GRAPHITE COMPOSITE MATERIAL FOR 3D PRINTING: A SUSTAINABLE ALTERNATIVE FOR THE PRODUCTION OF ELECTROCHEMICAL SENSORS FOR LEVOFLOXACIN

Amanda Garcia Batista (PG)*[1], Natália Marinho Caldas (IC)[1], Amanda de Souza Nicotte Silva (IC)[1], Dayenny Louise D'Amato Leite (PG)[1], Célia Machado Ronconi (PQ)[1], Lucas Vinicius de Faria (PQ)[2], Diego Pessoa Rocha (PQ)[3], Rafael Machado Dornellas (PQ)[1].

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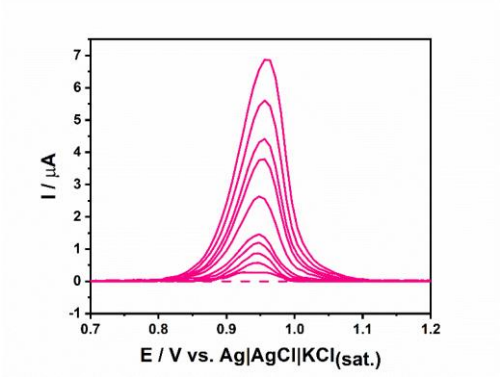
Palavras Chave:*PETG/graphite composite, Differential pulse voltammetry, Levofloxacin, 3D printing.,PETG/graphite composite,Differential pulse voltammetry,Levofloxacin,3D printing*

Highlights

Development of a low-cost PETG/graphite composite electrode for levofloxacin determination; Sensitive detection of LEV with LOD of 0.053 µmol L^{-1} and wide linear range (0.1–6.0 µmol L^{-1}).

Resumo/Abstract

The development of PETG-based composite materials has attracted increasing interest due to their low cost, mechanical strength, chemical resistance, and easy processing, enabling the fabrication of robust and versatile electrochemical platforms. In this context, a PETG/graphite composite was developed for the electrochemical determination of levofloxacin (LEV). Electrodes with different PETG:graphite ratios were prepared and characterized by X-ray diffraction (XRD) and Raman spectroscopy. Increasing graphite content enhanced crystallinity and decreased the ID/IG ratio, indicating improved graphitic ordering and fewer structural defects. These structural improvements resulted in a larger electroactive surface area, reduced charge-transfer resistance, and higher peak currents. The 60:40 (PETG:graphite) electrode exhibited the best electrochemical performance and was selected for analytical application. The electrochemical behavior of LEV at the optimized electrode was characterized in Britton–Robinson buffer (0.12 mol L^{-1}), with best response at pH 4.00. The dependence of peak potential on pH indicated the participation of protons in the oxidation process, suggesting a 1:1 electron–proton ratio in the rate-determining step. Scan rate studies revealed a mixed and irreversible process involving two electrons, allowing the proposal of a plausible oxidation mechanism. After optimization of differential pulse voltammetry parameters, a linear range from 0.1 to 6.0 µmol L^{-1} (r^2 = 0.998) was achieved, with detection and quantification limits of 0.053 and 0.10 µmol L^{-1}, respectively. The method showed good precision (RSD < 5%), selectivity against common interferents such as sodium lauryl sulfate, glucose, starch, and amoxicillin, and satisfactory recoveries (94–108%) in pharmaceutical samples, human serum, and synthetic saliva. Overall, the composite demonstrated enhanced conductivity, sensitivity, and reliability, confirming its potential as a low-cost and efficient platform for routine LEV determination.



Voltammograms of LEV (0.1–6 µmol L^{-1}) in 0.12 mol L^{-1} BR buffer pH 4.0.

Agradecimentos/Acknowledgments

The authors acknowledge CNPq, FAPERJ, and CAPES for financial support, as well as PGEB and PPGQ for institutional support

Nitrogen-Doped Carbon as a Platform for Ultra-Low-Cobalt, High-Performance HER Electrocatalysis

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Palavras Chave:*low metal loading,cobalt catalysts,active site selectivity,alkaline electrocatalysis,catalyst stability*

Highlights

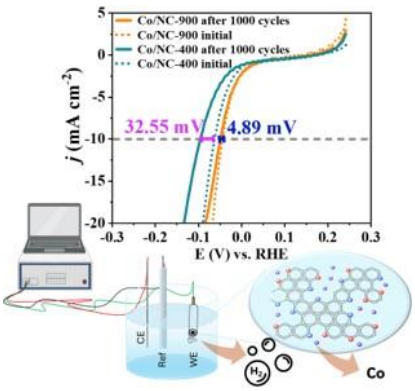
900 °C Co/N-doped carbon shows superior HER performance;

High HER activity achieved with minimal Co loading;

Selective Co-N active sites are more effective than higher metal content.

Resumo/Abstract

Two nitrogen-doped carbon materials (Na-NC) were synthesized by thermal treatment of cellulose at 400 and 900 °C in the presence of NaCl and hydrolyzed collagen as nitrogen source, aiming at the generation of negatively charged and well-defined nitrogen functionalities. Cobalt was subsequently incorporated by a room-temperature ion-exchange process. Despite its lower metal loading (0.10 wt% Co), the material treated at 900 °C (Co/NC-900) outperformed the sample synthesized at 400 °C (0.46 wt% Co), demonstrating that the formation of more selective and electronically favorable active sites is more effective than increasing the overall metal content. Electrocatalyst inks were prepared using a Nafion-containing water/isopropanol mixture and deposited onto glassy carbon electrodes for electrochemical evaluation. The hydrogen evolution reaction (HER) activity was investigated in alkaline medium (1 mol L^{-1} KOH) by linear sweep voltammetry. Co/NC-900 exhibited the best performance, with an onset potential of -0.012 V vs. SCE and an overpotential of -49 mV at 10 mA cm^{-2}, whereas Co/NC-400 required -102 mV to reach the same current density. These results highlight the critical role of high-temperature treatment in enhancing electrical conductivity and promoting more efficient cobalt-nitrogen coordination environments. In addition, Co/NC-900 demonstrated outstanding electrochemical stability, maintaining stable performance after 1000 potential cycles and during prolonged operation at 10 mA cm^{-2}, confirming that low loadings of earth-abundant transition metals can deliver high activity and durability when supported on properly engineered nitrogen-doped carbon matrices. Overall, this study demonstrates that rational control of surface chemistry enables highly active and durable HER electrocatalysts based on low loadings of earth-abundant transition metals, offering a sustainable and cost-effective strategy for hydrogen production in alkaline media.



N-doped carbon enables efficient HER with low cobalt loading.

Agradecimentos/Acknowledgments

We acknowledge financial support from FAPESP (Grant No. 2023/12949-7), Capes, CNPq, FINEP, and the LabIvo research group.

Nucleation and growth of silver films on PtRh metallurgical alloys in ethaline

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Palavras Chave:*Electrocrystallization,Electrodeposition,Deep eutectic solvents*

Highlights

The process of silver nucleation and growth on PtRh metallurgical alloys was influenced by temperature, resulting in progressive nucleation at 24 °C and instantaneous nucleation at 45 °C.

Resumo/Abstract

Focusing on electrolytic media, deep eutectic solvents (DES), which are mixtures of two or more compounds, such as choline chloride (ChCl) and ethylene glycol (EG), known as ethaline, are highlighted mainly because they can generate liquids with a melting point lower than that of their pure constituents. This work aimed to investigate the nucleation and growth processes of silver on Pt and PtRh metallurgical alloys ($Pt_{90}Rh_{10}$ and $Pt_{80}Rh_{20}$) at 24 °C and 45 °C. An electrolytic solution was prepared by combining ethaline (1ChCl:2EG) and 0.05 mol L^{-1} $AgNO_3$. In the electrochemical tests, a conventional three-electrode electrochemical cell was used, in which the electrodes consisted of Pt, $Pt_{90}Rh_{10}$, and $Pt_{80}Rh_{20}$ discs, with a geometric area of 6.36 × 10^{-3} cm^2 for Pt and 1.96 × 10^{-3} cm^2 for both alloys, respectively, Ag/AgCl/DES as the reference electrode, and a Pt plate as the auxiliary electrode. The electrodeposition experiments at both temperatures initially set a potential of 0.02 V for 10 s, followed by potential steps applied for 120 s. At 24 °C, potentials between −0.040 V and −0.060 V were applied for Pt and $Pt_{80}Rh_{20}$, and between −0.025 V and −0.050 V for $Pt_{90}Rh_{10}$; at 45 °C, the range of −0.010 V and −0.030 V was used for Pt, −0.015 V and −0.019 V for $Pt_{90}Rh_{10}$, and −0.010 V and −0.015 V for $Pt_{80}Rh_{20}$. According to the Scharifker and Hills' model for three-dimensional nucleation and growth under diffusional control, it was determined that increasing the temperature altered the nucleation mechanism, changing it from progressive to instantaneous, with an average value for the nuclei formation rate of 4.94×10^6 cm^{-2} s^{-1} at 24 °C and an average value for the total number of nuclei formed of 1.08×10^7 cm^{-2} at 45 °C. As expected, the effect of temperature promoted a change in the average value of the diffusion coefficient from 1.77×10^{-7} cm^2 s^{-1} at 24 °C to 2.21×10^{-7} cm^2 s^{-1} at 45 °C.

Agradecimentos/Acknowledgments

UFC, CNPq, CAPES, SECITECE FUNCAP-Rede VERDES, FINEP.

Palladium-doped g-C3N4 photoelectrocatalytic activity for ethanol electro-oxidation

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Palavras Chave:*Ethanol electro-oxidation, Photoelectrocalalysis, G-C3N4, Palladium*

Highlights

Pd-C_3N_4 for photoelectro-oxidation of etanol

Gains up to 230% of current after 1,5h

Resumo/Abstract

Here, we investigate carbon nitride doped with palladium (Pd-C_3N_4) for ethanol electro-oxidation in presence of light. A dispersion was prepared with 5mg of Pd-C_3N_4 in 1 mL of isopropyl and 10µL of Nafion. Subsequently, 20 µL of this dispersion was drop-casted onto a glassy carbon electrode. After drying, the working electrode was submitted to 100 voltammetric cycles at 150 mVs^{-1} in presence of aqueous 0.1 M KOH for cleaning/conditioning the surface.

Afterwards, cyclic voltammograms were collected in a 0.1 M KOH + 1.0 M ethanol solution under dark and light conditions. For that we used a full spectrum LED of 50 W, with an emission gap of 400-840nm. Under lighting, the initial performance of Pd-C_3N_4 for ethanol electro-oxidation was 57% higher (in terms of peak currents) when compared to dark conditions. Chronoamperometry was performed for 2 h at 0.7 V to evaluate the stability of the photoelectrocatalytic response of the film. After 1.5 h, the current gain reached 230%. Subsequently, new voltametric cycles were obtained, and the peak current gain was ~ 82%.

X-ray diffraction analysis indicates that Pd is present in both metallic and oxide forms. Based on the values obtained, the catalyst is polycrystalline, with predominance of planes (111) and (200).

In situ FTIR spectra in the dark show bands at 1086 and 1049 cm^{-1} related to ethanol consumption, and at 1547 and 1411 cm^{-1}, which indicate the production of acetate. Under illumination, spectra show a growing band centered at 2344 cm^{-1}, corresponding to the production of CO_2. It is noteworthy that this band emerges only at potentials as high as 1.0 V, which indicates that CO_2 generation is a late-stage process.

Summarizing, Pd-C_3N_4 exhibits photoelectrocatalytic activity for ethanol oxidation, generating acetate as the main oxidation product. The results under light remain inconclusive, necessitating further refinement and stabilization of the spectral region between 2000 and 1500 cm^{-1}.

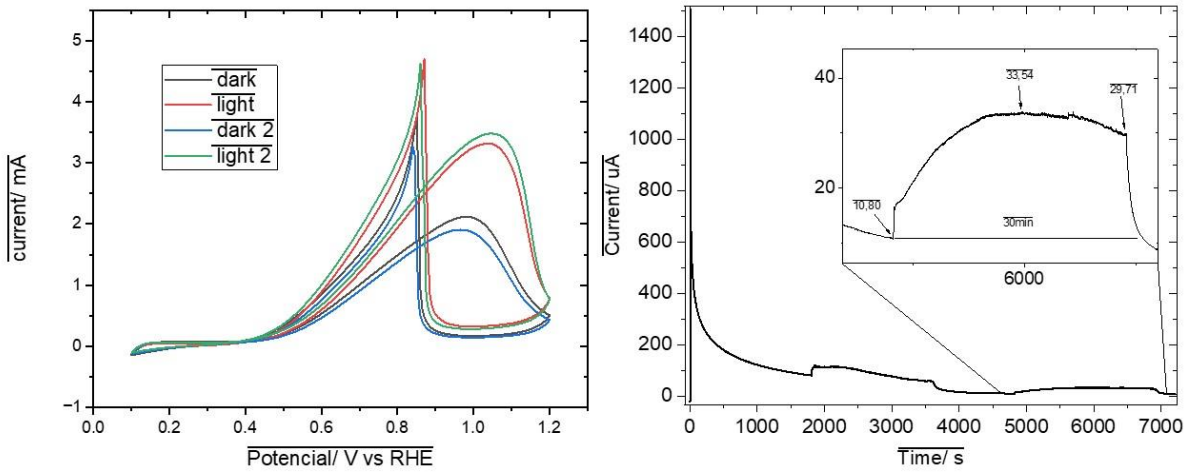


Figure 1. Voltametric profile of Pd-C3N4 in KOH 0,1M + ethanol 1,0M and Chronoamperometry at 0,7 V.

Agradecimentos/Acknowledgments

PROPP/UFMS, CAPES, CNPq, FINEP, FUNDECT and CAPES for financial support

Pencil graphite electrodes modified with in situ graphite oxide applied to the electrochemical study of dexamethasone

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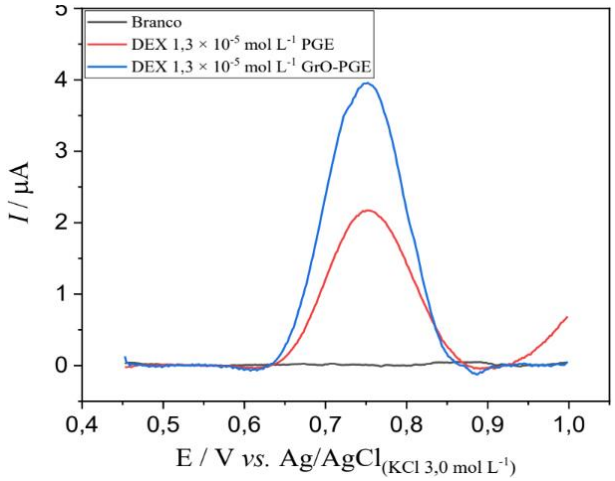
Palavras Chave:*Dexamethasone,dexamethasone,Electroanalytical,Graphite pencil electrode,modified electrodes*

Highlights

*In situ*modification of pencil graphite electrode;
Greater repeatability and signal intensity of DEX after electrogeneration of graphite oxide;
Affordable, low-cost electrodes for DEX determination.

Resumo/Abstract

The monitoring of pharmaceuticals in natural waters is relevant due to potential environmental and public health impacts, requiring sensitive and practical analytical methods. The aim of this work was to develop and characterize pencil graphite electrodes (PGE) modified by*in situ*graphite oxide electrogeneration (GrO-PGE) for the electrochemical quantification of dexamethasone (DEX) in natural waters. The modification of the PGEs was performed using HB and H graphite pencils, applying five consecutive scan cycles in the potential range from −0.1 V to +2.1 V, with a scan rate of 50.0 mV s^{-1}, in 0.1 mol L^{-1} phosphoric acid. The GrO-PGEs were characterized by scanning electron microscopy (SEM) and cyclic and square wave voltammetry. SEM micrographs revealed a more irregular and rough surface for the H graphite electrode, indicating partial oxidation of the graphite layers and an increase in the electroactive area, which corroborated the voltammetric results. The H-type GrO-PGE showed better results in terms of sensitivity and repeatability for DEX quantification. Cyclic voltammetry showed that DEX presents an irreversible reduction peak controlled by adsorption at −0.9 V vs. Ag/AgCl and a quasi-reversible oxidation peak at +0.8 V, dependent on the reduction peak. Square-wave adsorptive stripping voltammetry analyses indicated a 1.8-fold increase in the peak current of DEX over GrO-PGE, attributed to improved charge transfer promoted by graphite oxide. Repeatability was evaluated at three concentrations levels (5.0×10^{-6}, 9.1×10^{-6}, and 1.3×10^{-5} mol L^{-1}) in triplicate, with a significant reduction in RSD after modification, from 2.88–34.51% (PGE) to 5.89–7.35% (GrO-PGE). The results demonstrate that GrO-PGE is an effective strategy for increasing the sensitivity and reliability of electroanalytical methods applied to the quantification of DEX in natural waters, combining simplicity, speed, and low cost.



Cyclic voltammograms of 1.3 x 10 $^{-5}$ mol L $^{-1}$ DEX on PGE and GrO-PGE (B-R buffer 0.1 mol L $^{-1}$, pH 2)

Agradecimentos/Acknowledgments

CAPES, FAPESP, CNPq, UNIFESP PPGQ-CTS, LABEE-BIA.

PET-based screen-printed electrodes modified with AuNPs and carbonaceous materials

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Palavras Chave:*Silk Screen,Metallic Nanoparticles,Carbon ink*

Highlights

Electrochemical sensor based on modified PET substrates; Synergistic effect of carbon and gold nanoparticles (AuNPs) for sensing; Low-cost fabrication process for mass production; Device for PoC testing.

Resumo/Abstract

Screen-Printed Electrodes (SPEs) represent an efficient alternative to conventional electrochemical systems, due to their cost-effectiveness and fabrication simplicity. These devices can be mass-produced through printing techniques such as silk-screening, using conductive inks applied onto various substrates, ensuring economic viability. The incorporation of carbonaceous materials decorated with gold nanoparticles (AuNPs) provides a suitable microenvironment for biomolecule immobilization, promoting an enhanced electrochemical response with high sensitivity and specificity. The construction of PET-based screen-printed electrodes followed a protocol described in the literature [Ferreira et al., 2023]. The conductive ink was prepared using varying proportions of graphite, commercial nail polish (as a binder) and cyclohexanone. The working electrodes were fabricated by the screen-printing method on PET substrates. The AuNps were obtained using as the metallic precursor $HAuCl_4$ (3,0 mmol L^{-1}), $NaBH_4$ (6,0 mmol L^{-1}) as reducing agent, and 3-n-propylpyridinium silsesquioxane chloride ($SiPy^+Cl^-$4 g L^{-1}) as stabilizing agent. To obtain the nanohybrid materials, silsesquioxane-stabilized AuNPs were drop-casted onto the surface of SPE. Optimization of the ink composition revealed that SPE prepared with a ratio of 70% graphite, 30% binder, and 150% cyclohexanone exhibited superior voltammetric behavior in presence of the redox probe $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$, characterized by higher peak currents and reduced peak-to-peak separation (ΔE_p= 0,488 mV). SPEs obtained under these conditions displayed an electroactive area of 3,2 mm^2 and a diffusion-controlled process (log I vs log n, R^2= 0,9623). The incorporation of stabilized AuNPs promoted a significant increase in current signals, enhancing the sensitivity of the devices and enabling biomolecule immobilization for the development of point-of-care (PoC) systems.

FERREIRA, L.M.C. et al. Talanta Open, v. 7, 100201, 2023.

Agradecimentos/Acknowledgments

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Photoelectrochemical CO2 reduction using Cu2WO4 modified with polysiloxane in gas-diffusion electrodes

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Palavras Chave:*CO2 reduction reaction, Gas diffusion electrode, Copper (I) tungstate, Photoelectrochemistry, Protective layers,CO2 reduction reaction,Gas diffusion electrode,Copper (I) tungstate,Photoelectrochemistry,Protective layers*

Highlights

Cu_2WO_4 gas-diffusion electrode produced ethanol from photoelectrochemical CO_2 reduction; modification with polysiloxane inhibited the semiconductor degradation and increased the electrode stability.

Resumo/Abstract

The emission of CO_2 in the atmosphere has been increasing in the last two centuries. However, this greenhouse gas can be converted to value-added products using solar energy and semiconductor electrodes.

This contribution presents the investigation of Cu_2WO_4 electrodes for application as photocathodes for photoelectrochemical CO_2 reduction reaction (PEC-CO_2RR) under solar-simulated irradiation (100 mWcm^{-2}) in CO_2-saturated $NaHCO_3$ aqueous solution. First, Cu_2WO_4 particles were deposited on carbon paper (C_p) or glass-FTO; then, the electrode surface was modified with a film of an amine-functionalized polysiloxane (AF-PSi) dissolved in THF. UV-Vis absorption spectroscopy revealed that AF-PSi solutions with concentration greater than 1 mg/L significantly changed the optical properties of FTO|Cu_2WO_4/AF-Psi. Electrochemical measurements were first carried out for electrodes prepared using glass-FTO as substrate. Then, using carbon paper as substrate, CO_2-fed C_p/Cu_2WO_4/AF-PSi (as well as, C_p/Cu_2WO_4) was used as gas diffusion electrodes in PEC-CO_2RR. After a 2h-electroysis performed under potentiostatic control at – 0,3 V vs. Ag/AgCl, analysis of the electrolyte revealed 5,21 µM of ethanol produced from PEC-CO_2RR for both the electrodes. The morphology of the electrodes surface was examined by SEM; while the surface of unmodified electrode was damaged, the surface of C_p/Cu_2WO_4/AF-PSi remained unaltered. The performance and long-term stability of these electrodes in non-aqueous electroyte is under investigation.

Agradecimentos/Acknowledgments

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Physicochemical Characterization of 3D-Printed Hollow Carbon Paste Microneedle Electrodes for Electrochemical Interface Studies

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Palavras Chave:*Microneedle Electrodes,3D Printing,Electrochemical Interfaces,O_2 Plasma Treatment,Physicochemical Characterization.*

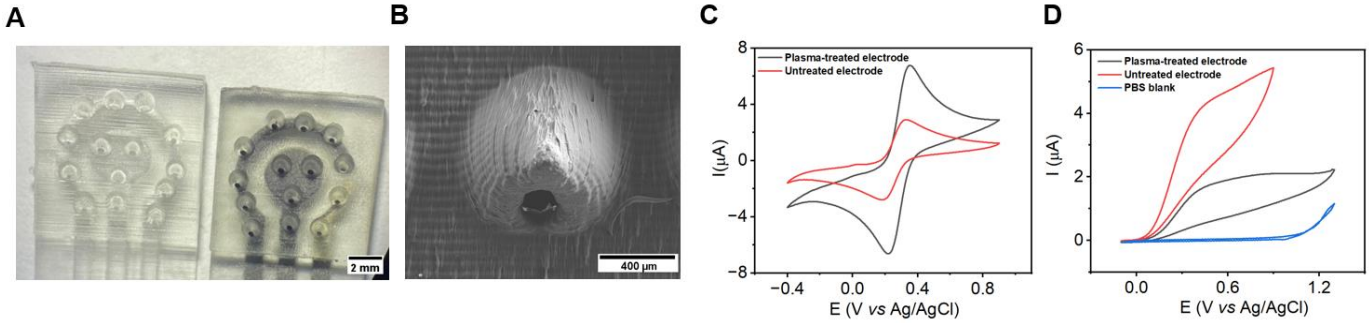
Highlights

3D-printed hollow carbon paste microneedle electrodes exhibit enhanced hydrophilicity, improved electrochemical accessibility, and modulated interfacial charge transfer after O_2 plasma treatment.

Resumo/Abstract

In this work, the development and characterization of a hollow microneedle electrode containing carbon paste are presented, with the aim of applications in electroanalysis and the study of electrochemical interfaces. The device was designed using three-dimensional modeling and fabricated by 3D printing, comprising hollow microneedles with a height of 1.5 mm, a base diameter of 1.0 mm, and an internal channel diameter of 0.57 mm for filling with conductive carbon ink. This geometry results in an integrated three-dimensional architecture inspired by screen-printed electrodes. Morphological characterizations by optical microscopy and scanning electron microscopy confirmed the good geometric definition of the microneedles, the structural integrity of the hollow microchannels, and the homogeneous distribution of the conductive material. Mechanical compression tests showed that incorporating the carbon paste does not compromise the array's mechanical strength, preserving properties compatible with minimally invasive applications.

Surface modification by O_2 plasma promoted a significant reduction in the contact angle, indicating increased surface hydrophilicity and favoring the electrode/electrolyte interaction within a microstructured architecture. The electrochemical response was investigated using the $[Fe(CN)_6]^{3-/4-}$ and $[Ru(NH_3)_6]^{3+/2+}$ redox couples in different electrolytes. The $[Ru(NH_3)_6]^{3+/2+}$ couple, characteristic of outer-sphere electron-transfer processes, exhibited highly reproducible electrochemical behavior, with reduced charge-transfer resistance and increased electroactive area after plasma treatment, evidencing improved electrochemical accessibility and enhanced connectivity of the conductive phase. For the $[Fe(CN)_6]^{3-/4-}$ couple, which is more sensitive to interfacial conditions and electrolyte composition, an enhanced response was also observed after treatment, consistent with improved wetting and interfacial accessibility despite its anionic nature.



(A) Optical images (B) SEM images (C) CV of the [Fe(CN)6]3-/4- (D) CV ascorbic acid oxidation in PBS

Agradecimentos/Acknowledgments

This work was supported by FAPESP, CNPq, INCTBio-LK, and CAPES.

Plasmonic Contributions to the CO2 Reduction Reaction: An In Situ/Operando Study

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Palavras Chave:*XANES,FTIR,CO2 reduction,electrocatalysis,plasmonics*

Highlights

Shape-dependent Cu reduction profiles via*operando*XANES.

Laser delays reduction, distinguishable from thermal effects.

Enhanced HCO_3^- adsorption and H_2O desorption under plasmonic excitation.

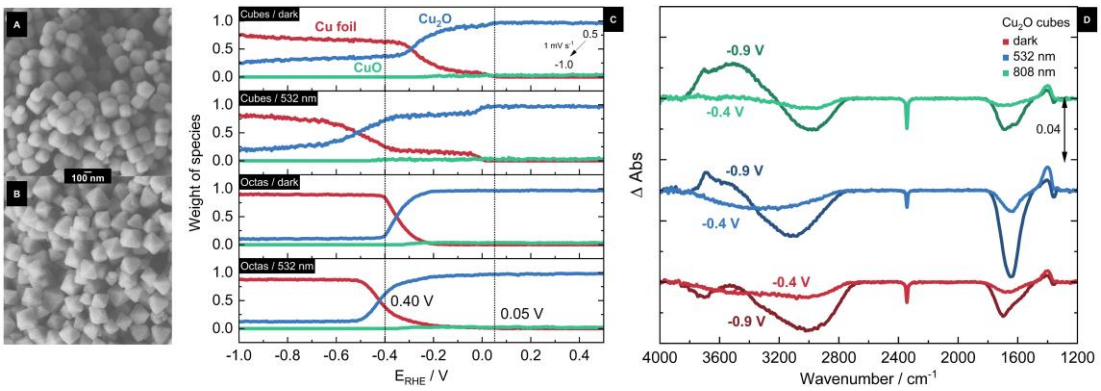
Resumo/Abstract

Electrochemical CO_2 reduction (CO_2RR) reduces atmospheric CO_2 and incentivizes sequestration. Cu_2O-derived catalysts excel for longer carbon products, with controllable shapes (cubes or octahedra). Laser illumination boosts activity via plasmonics, but studies rarely distinguish heating from hot electron effects; interface dynamics are crucial for improvements. This work examines plasmon-assisted CO_2RR in 0.1 M $KHCO_3$: electrolyte interface via*in situ*FT-IRRAS and catalyst oxidation via*operando*XANES, using Cu_2O cubes (Fig. A) and octahedra (Fig. B).

Fig. C shows linear combination analysis of*operando*XANES spectra during slow LSV for CO_2RR, with/without 532 nm laser illumination. Reduction profiles differ: cubes exhibit two regions (0.05 V and ~0.3 V, potentials referred to RHE), octahedra show one (~0.2 V), indicating distinct reactivity sites. In both, laser delays Cu reduction by several mV and creates plateaus, suggesting a well-defined separation of the processes.

Fig. D shows*in situ*FT-IRRAS for Cu_2O cubes under varied illuminations to assess temperature impacts at two potentials: 532 nm induces plasmonics, 808 nm only photothermal effects. Common features: H_2O/CO_2 ad/desorption (O-H stretch 3000-3600 cm^{-1}, H-O-H bend 1600 cm^{-1}), diluted CO_2 at 2343 cm^{-1}, HCO_3^-/CO_3^{2-} adsorption at 1400 cm^{-1}. Rapid CO_2 consumption and equilibration at -0.4 V, with H-bond breakage seen by negative H_2O bands. At -0.9 V, H_2O desorbs in the "ice-like" structure (3000 cm^{-1}) while adsorbs in the "liquid-like" (3500 cm^{-1}). It is also possible to observe “free O-H” bands around 3700 cm^{-1} which is suggestive of a surface with low quantity of H-bonds. This is especially noticeable with the 532 nm laser, which also presented higher desorption of H_2O in the bending region and stronger adsorption of HCO_3^-/CO_3^{2-}.

In summary, plasmonic illumination modulates Cu reduction and interface via hot electrons. This enables tailored Cu_2O for better selectivity/efficiency in carbon mitigation.



A and B: Cu2O cubes and octahedra SEM images. C: Oxidation state by XANES. D: FTIR spectra.

Agradecimentos/Acknowledgments

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Polyaniline/MoS2 nanocomposite thin films for transparent and electrochromic energy storage devices

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Palavras Chave:*Molybdenum Disulfide,Polyaniline,Energy Storage,Electrochromism*

Highlights

Synthesis, characterization and electrochromic evaluation of polyaniline/MoS_2 nanocomposite thin films, prepared via liquid-liquid interfacial route.

Resumo/Abstract

Over the past decades, renewable energy production has risen massively, leading to a greater usage of electrochemical energy storage devices, which are constantly being improved. The shift from organic to aqueous devices, specifically, has attracted a lot of attention and boosted the development of new materials for their construction. Two materials that have been heavily researched for such application are polyaniline (PAni) and Molybdenum Disulfide (MoS_2), due to their great electrical and optical properties, that are also tunable, as well as their low environmental impact. Polyaniline is also interesting because its three different oxidation states grant it pronounced electrochromic properties, shifting through various colors over a large potential window, which can be paired with energy storage for a myriad of interesting applications. With that, this work deals with the preparation of composites between polyaniline and MoS_2, varying the ratio between the two, via the liquid-liquid interfacial route (LLIR). This route provides a simple and elegant way of obtaining complex materials, already processed in the form of thin, transparent and highly homogeneous films, that can be deposited over any subtract of interest. [1] The obtained films were characterized by UV-Vis and Raman spectroelectrochemistry, SEM, cyclic voltammetry and galvanostatic charge-discharge curves. All films displayed characteristic supercapacitor behavior, with the composites showing improved electrochemical properties, when compared to neat polyaniline and MoS_2, with increased cycle stability and volumetric capacitances achieving values over 450 F cm^{-3}. Finally, varying the ratio between PAni and MoS_2resulted in an improvement in the electrochromic properties of polyaniline, by allowing a more complete transition between its oxidation states, which also contributed to a higher volumetric capacitance in such films.

[1] ZARBIN, Aldo J. G. Materials Horizons,**8**, 1409-1432 (2021)

Agradecimentos/Acknowledgments

CAPES, CNPq, INCT-Nanocarbono and INCT-NanoVida.

Polypyrrole-Coated Microneedles for Offline Electrochemical Detection of Interferon-Alpha in Interstitial Fluid

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Palavras Chave:*Microneedles;,Polypyrrole;,Electrochemical biosensor;,Interferon-alpha;,Interstitial fluid;*

Highlights

Conductive polypyrrole-coated microneedles enable label-free, offline electrochemical detection of IFN-α in interstitial fluid with high sensitivity and mechanical robustness.

Resumo/Abstract

Monitoring cytokines such as interferon-alpha (IFN-a) is crucial for evaluating immune responses during viral infections, autoimmune disorders, and immunotherapies. In this work, we report the development of a minimally invasive microneedle-based electrochemical biosensor for the offline, label-free detection of IFN-α in interstitial fluid (Figure 1). Polycaprolactone (PCL) microneedle arrays were fabricated using 3D-printed molds and thermocompression, and subsequently coated with polypyrrole (PPy) via in situ oxidative polymerization, thereby providing electrical conductivity and a suitable interface for biomolecule immobilization. The influence of PPy concentration (10–200 mmol·L^{-1}) on morphology, porosity, mechanical performance, and electrochemical behavior was systematically investigated. An intermediate PPy content (50 mmol·L^{-1}) was identified as optimal, yielding enhanced surface roughness, increased porosity (~30%), enlarged electroactive area, and improved charge-transfer properties while preserving mechanical integrity and insertion capability. Electrochemical characterization using cyclic voltammetry and impedance spectroscopy demonstrated a sensitive response to IFN-α, with a detection limit of 8.6 pg·mL^{-1} and a linear range up to 1000 pg·mL^{-1}. The biosensor exhibited high specificity for IFN-α in the presence of interfering cytokines and proteins, and its performance was validated in gelatin-based matrices that mimicked interstitial fluid. Cytotoxicity assays using keratinocyte and fibroblast cell lines confirmed the biocompatibility of the PPy-coated microneedles. The sensing strategy operates through skin insertion, immunocapture of the target analyte, and subsequent electrochemical readout after device removal, enabling robust offline analysis without complex instrumentation. These results demonstrate that PPy-coated microneedles are a scalable and minimally invasive platform for cytokine monitoring and point-of-care diagnostics.

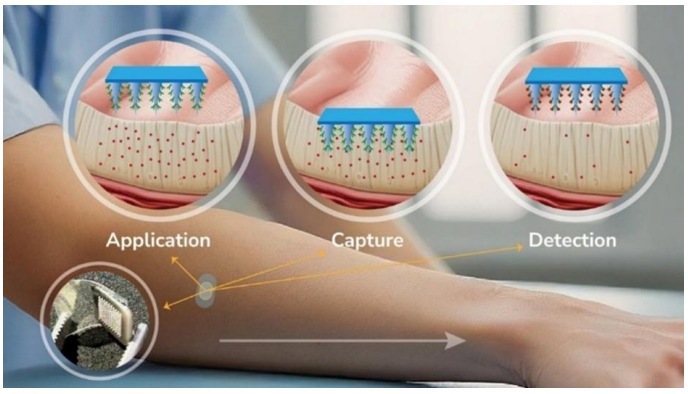


Figure 1. Microneedle-based biosensing process with offline electrochemical detection.

Agradecimentos/Acknowledgments

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Printed electrodes modified with Ni/Mg/Al-carbonate layered double hydroxide: an electrochemical interface study

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Palavras Chave:*Electrochemistry,Chitosan,Film,Graphite,Interfacial*

Highlights

Printed electrodes modified with HDL-NiMgAl–CO_3^{2-} reveal strong interfacial reconfiguration even in neutral electrolyte.

Resumo/Abstract

Layered double hydroxides (LDHs) have been used as electrode modifiers for energy storage and electrocatalysis[1,2]. However, aspects related to the interface architecture of these materials lack investigation. In this work, the electrochemical behavior of commercial printed electrodes modified with NiMgAl–CO_3^{2-} LDH, graphite (C), and chitosan (CS) was evaluated, focusing on the influence of the film on the electrochemical response of the system. Electrochemical characterization was performed by cyclic voltammetry in $Fe(CN)_6^{3-}/^{4-}$ (0,01M) and KCl (0,50M) solution, at different scan rates, analyzing changes in reversibility and charge transfer. Different proportions between graphite and LDH were evaluated, maintaining the polymeric matrix as a stabilizing element. The voltammograms show an increase in peaks, a shift in peak potentials, and an increase in capacitive current, even in compositions with a higher graphite fraction, demonstrating that LDH acts as an active modulator of the electrode/electrolyte interface, affecting the apparent kinetics of the system through interface processes associated with the hybrid matrix and the formation of local alkaline microenvironments. Note that the increase in graphite favors electron transport without eliminating chemical and structural effects of the film. Therefore, the results suggest that the electrochemical response is governed by the optical fiber between electron transfer and interfacial processes, and not only by the presence of redox-active species.

[1]RAY, Priyadarshi K.; PARIDA, Kulamani. Achievements, challenges, and stability of layer double hydroxide and carbon nanotube hybrid electrode materials for clean and sustainable energy storage supercapacitor application: an extensive review.**Materials Advances**, v. 6, n. 1, p. 84-116, 2025.

[2]BARI, Bushra; TYAGI, Pawan; UDEOCHU, Uche. Cyclic voltammetry insights into Ni/Al-carbonate hydrotalcite catalysis for methanol oxidation.**Scientific Reports**, v. 15, n. 1, p. 13365, 2025.

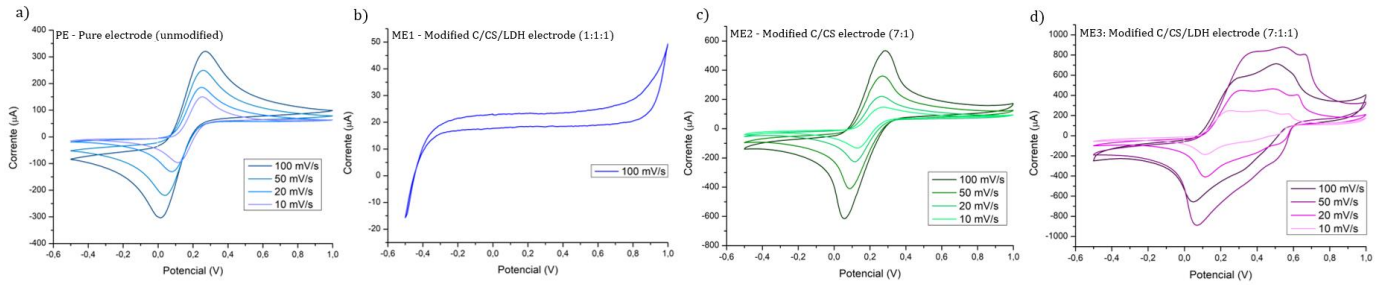


Figure 1: Voltammograms: a) Pure electrode, b) C/CS/LDH (1:1:1), c) C/CS and d) C/CS/LDH (7:1:1).

Agradecimentos/Acknowledgments

We thank FAPERJ, CNPq, and CAPES.

Salt-assisted pulsed laser ablation in liquids for engineering nanomaterials toward electrochemical sensing

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Palavras Chave:*Green synthesis,Electrochemical sensing,Pulsed laser ablation in liquid,Nafion®-modified electrodes,Surface functionalization*

Highlights

Green, ligand-free synthesis of GQDs and AuNPs via salt-assisted pulsed laser ablation in liquid. Saline media enable controlled surface chemistry and tunable electrochemical properties.

Resumo/Abstract

This work reports the synthesis of ligand-free gold nanoparticles (AuNPs) via pulsed laser ablation in liquid (PLAL) in saline electrolytes (NaCl, NaNO3, Na2SO3) for electrochemical serotonin (5-HT) sensing. The saline medium modulated AuNP properties: sulfite anions enhanced colloidal stability via electrostatic interactions, nitrate promoted surface oxidation states ($Au1^{+}$/$Au3^{+}$), and chloride-sulfite mixtures reduced particle size. Comprehensive characterization confirmed AuNPs with tailored dimensions, minimized aggregation, and tunable surface chemistry. A glassy carbon electrode (GCE) modified with NaNO3-derived AuNPs (N-AuNPs) embedded in Nafion® exhibited enhanced electrocatalytic activity for 5-HT oxidation compared to an unmodified GCE. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) revealed improved interfacial kinetics and charge transfer at the N-AuNPs/Nafion®/GCE. Under optimized differential pulse voltammetry (DPV) conditions (pH 6.0), the sensor displayed a linear response to 5-HT from 0.1 to 25.0 µmol L^{-1} (R2 = 0.9991) with a detection limit of 20 nmol $L^{-}1$. Selectivity was validated against serum interferents, showing <15 % signal variation. The sensor demonstrated excellent repeatability (intra-day RSD 4.8 %, inter-day RSD 7.6 %) and robust recovery (104–108 %) in simulated serum. The new electrochemical platform N-AuNPs/Nafion®/GCE demonstrated promising characteristics for application in biological and/or pharmaceutical analysis.

Agradecimentos/Acknowledgments

CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico; Fundação de Apoio à Pesquisa e Inovação do Estado de Santa Catarina – FAPESC; CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior)

Sensor eletroquímico molecularmente impresso para determinação de ácido propiônico em biorreatores anaeróbicos

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Palavras Chave:*Ácido proprionico, L-treonina, Óxido de grafeno reduzido. Sensor eletroquímicos. Biogás. Ácidos graxos.,L-treonina, Óxido de grafeno reduzido. Sensor eletroquímicos. Biogas. Ácidos graxos.*

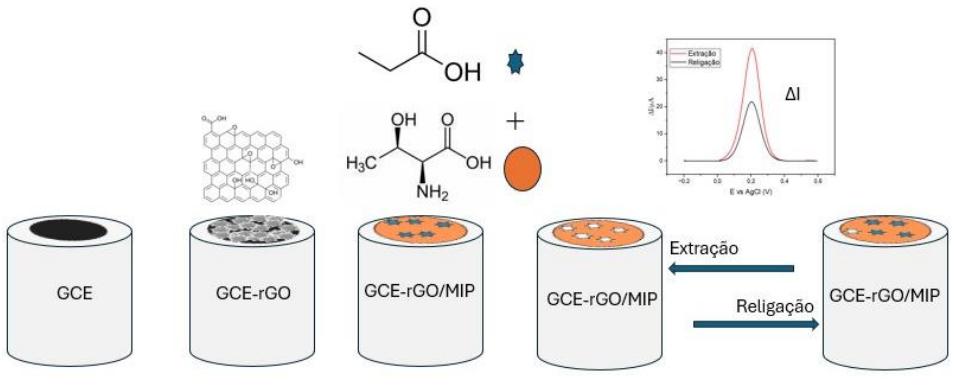
Highlights

A molecularly imprinted electrochemical sensor was developed for PA detection. rGO was co-deposited on GCE with MIP to enhance imprinted site locations and sensor sensitivity.

Resumo/Abstract

O biogás, biocombustível da decomposição anaeróbica de biomassa, é alternativa sustentável aos fósseis, alinhada aos ODS da ONU sobre clima. Porém, a formação de ácido propiônico (AP) causa instabilidade do reator e queda na produção de metano. Métodos tradicionais como HPLC e GC-FID apesar de sensíveis, são caros e demandam preparo de amostra. Diante disso, o desenvolvimento de um sensor eletroquímico que tenha resposta rápida, alta sensibilidade, portabilidade e baixos limites de detecção torna-se atrativo. Assim, este trabalho tem por objetivo desenvolver sensores eletroquímicos modificados com óxido de grafeno reduzido (rGO) e polímero molecularmente impresso (MIP) para monitorar AP em biorreatores. Para construção do sensor foi utilizado eletrodo de carbono vítreo (GCE) como eletrodo de trabalho, $Ag/AgCl_{sat}$ como referência e um fio de platina como auxiliar. O rGO foi eletrodepositado no GCE por cronoamperometria, no potencial de -1,5 V por 500 segundos, como descrito anteriormente [1]. Na construção do MIP, foi utilizado o monômero L-treonina (1×10^{-4}mol/L) e AP (5×10^{-5} mol/L) em PBS 0,2 mol/L pH 6, por voltmetria cíclica (CV) na faixa de potencial de -0,5 a 1,5 V, durante 12 ciclos. As respostas de corrente foram avaliadas em uma solução de 5×10^{-3}mol/L de $Fe(CN)_6^{4-/3-}$ em 0,10 mol/L, usada como sonda redox. Após a eletropolimerização observou-se queda de corrente devido à formação do filme de politreonina, que dificultou a transferência eletrônica. Após extração do analito em etanol/ácido acético (9:1 v/v), observou-se aumento de corrente devido à formação de cavidades impressas no filme. Para religação, o eletrodo foi imerso em solução de AP e foi observado uma queda de corrente sugerindo que algumas cavidades foram ocupadas pelo analito. Portanto, esses resultados mostram que o sensor é promissor para monitorar a presença de AP em bioreatores durante a produção de biogás.

[1] M. A. Beluomini, et al.*Talanta*, vol. 165, pp. 231–239, Apr. 2017.



Etapas da modificação do GCE com rGO e L-treonina contendo AP para formação de MIP.

Agradecimentos/Acknowledgments

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Sensores eletroquímicos miniaturizados: da fabricação à aplicação em sistemas reais

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Palavras Chave:*validação analítica,serigrafia,monitoramento ambiental,detecção em estado sólido,eletrodos descartáveis*

Resumo/Abstract

Sensores eletroquímicos têm sido amplamente desenvolvidos devido ao seu baixo custo, portabilidade e capacidade de detectar e quantificar diferentes substâncias em diversas matrizes, muitas vezes em tempo real. No entanto, ainda existem desafios significativos para sua transição do laboratório para o mercado. Nesta miniconferência, serão discutidas estratégias de fabricação e validação analítica de sensores eletroquímicos que vêm sendo implementadas pelo Laboratório de Espectroanalítica, Eletroanalítica e Sensores (IQ-UFG), com o objetivo de contribuir para a viabilidade desses dispositivos. Também serão apresentadas novas estratégias para a detecção de analitos em estado sólido, bem como alternativas para detecção multiplexada em células eletroquímicas convencionais.

Agradecimentos/Acknowledgments

CAPES, CNPq (441854/2023-0, 403306/2023-0), FAPEG, UFG, EMATER, Centro de Excelência em Saúde Única (CESU)

Shape-Controlled Gold Nanoparticles at Carbon Interfaces for Electrochemical SERS Detection of Pesticides

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Palavras Chave:*carbon interfaces,gold nanoparticles,vibrational spectroscopy,SERS,pesticide*

Highlights

Pesticide use raises environmental and health concerns, driving the need for sensitive, specific detection. Combined electrochemical-SERS platforms enable simultaneous modulation and characterization.

Resumo/Abstract

The widespread application of pesticides in contemporary agriculture has intensified concerns related to environmental contamination and human health, highlighting the need for analytical strategies capable of providing high sensitivity and molecular specificity. In recent years, platforms that combine electrochemical techniques with surface-enhanced Raman spectroscopy (SERS) have emerged as powerful tools, as they enable simultaneous electrochemical modulation and vibrational characterization of target molecules. The shape-controlled gold nanoparticles used in this study, exhibiting high stability, were synthesized and characterized by UV-vis spectroscopy and transmission electron microscopy prior to the electrochemical SERS investigations. References:

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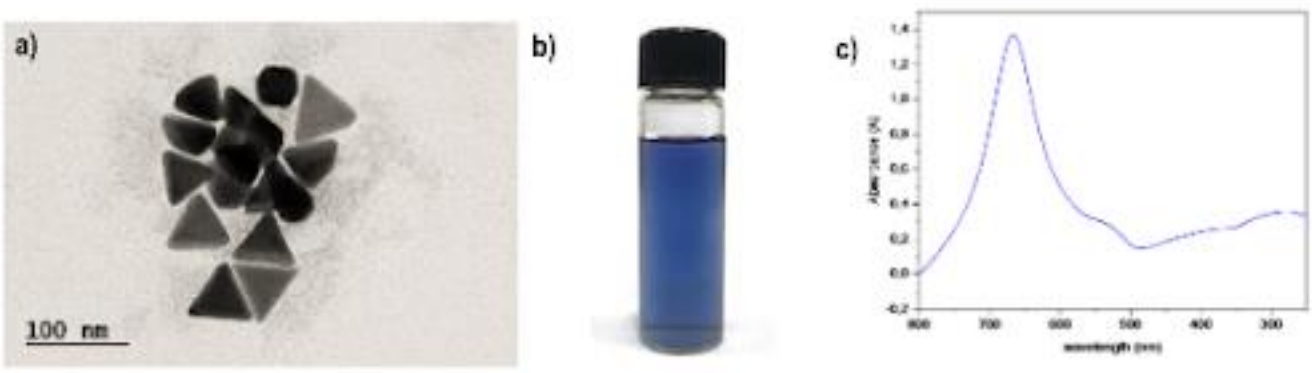


Figure 1. a) TEM image of AuNPs; b) AuNP suspension; c) UV-vis extinction spectrum

Agradecimentos/Acknowledgments

We acknowledge support from CAPES, CNPq and FAPESP (2025/27044-5 e 2025/14249-8)

Simultaneous production of green H2 using a hybrid electrolyzer for the treatment of industrial effluents to produce electrical energy with Fuel Cell

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Palavras Chave:*Fuel cell,Green hydrogen,wastewater treatment,electrochemical oxidation*

Highlights

A hybrid electrochemical system simultaneously treats dye-contaminated effluents and produces green hydrogen with energy recovery via a fuel cell

Resumo/Abstract

This work evaluates a hybrid electrochemical system applied simultaneously to the treatment of industrial effluents and the production of green hydrogen, with subsequent conversion into electrical energy through a fuel cell. The study was carried out using a synthetic effluent contaminated with methyl red dye, submitted to an advanced electrochemical oxidation process in a PEM-type reactor operating in batch mode. Dye degradation occurred in the anodic compartment, while hydrogen was generated in the cathodic compartment and collected for quantification and energy use. Different electrolytes (H2SO4, Na2SO4, and NaOH) and current densities (80, 100, and 150 mA cm^{-2}) were evaluated, analyzing their influence in the contaminant degradation, hydrogen production, and electrical energy generation. Parameters such as pH and electrical conductivity were used to support the evaluation of the electrochemical process efficiency. The results demonstrated that acidic medium (H_2SO_4) and higher current density favored both dye degradation and hydrogen production, reaching volumes of up to 3540 mL and a maximum electrical generation of 11.8 W. The integration of the electrolyzer with a fuel cell evidenced the feasibility of converting the produced hydrogen into electrical energy in a stable manner. Thus, this study highlights the potential of hybrid electrochemical processes as a sustainable alternative to combine environmental remediation, green hydrogen production, and energy recovery.

Agradecimentos/Acknowledgments

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Structural Evolution and Catalytic Insights into Cobalt Spinel Oxide for Electrochemical Ammonia Production

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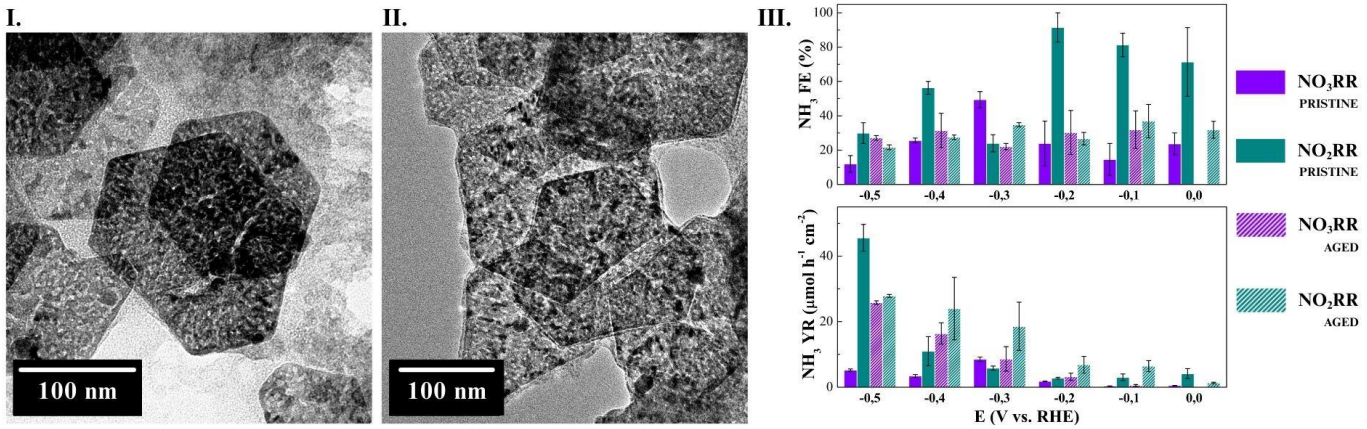
Palavras Chave:*Ammonia electrosynthesis,NO3RR,NO2RR,Co3O4 nanoplates,Electrocatalyst stability.*

Highlights

Surface restructuring of Co_3O_4 nanoplates after accelerated electrochemical aging enabled sustainably higher ammonia production rates.

Resumo/Abstract

In a scenario where NH_3 production via the Haber-Bosch process intensifies environmental impacts, electrocatalytic ammonia synthesis emerges as a sustainable alternative. This approach further converts pollutants (NO_3− and NO_2−) into a commodity. In this context, the performance of cobalt oxide nanoplates was evaluated for both short- and long-term operation in nitrate and nitrite reduction reactions. XRD confirmed the cubic spinel phase and SEM/HRTEM evidenced a morphology of ultrathin hexagonal nanoparticles (Figure I), while XPS analysis revealed Co^{3+}/Co^{2+} ratio of approximately 1:1. The electrochemical measurements were performed in an H-type cell using 0.2 mol L^{-1} $NaNO_3$ or $NaNO_2$ in 1.0 mol L^{-1} NaOH with Co_3O_4-np serving as the catalyst. The catalyst showed a high Faradaic Efficiency of 92.5 ± 7.5% at −0.2 VRHE and a Yield Rate of 45.6 ± 4.1 µmol h^{-1} cm^{-2} at −0.5 VRHE during NO_2− reduction, as well as a FE of 49.4 ± 0.5% and a YR of 8.5 ± 0.6 µmol h^{-1} cm^{-2} at −0.3 VRHE during NO_3− reduction (Figure III). The product quantification and origin were validated by NMR. The Co_3O_4-np underwent accelerated electrochemical aging over 1000 CV cycles resulting in decreased NH_3 FE and increased YR, attributed by DRT analysis to enhanced electron-transfer kinetics due to reduced resistance. Both*online*ECMS and DFT techniques demonstrated that the loss of selectivity resulted from increased competition with the HER after cycling. Furthermore, microstructural characterization revealed increased nanoplate length and formation of an amorphous phase on edges (Figure II), while XPS spectra showed an increased Co^{3+}/Co^{2+} ratio. Consequently, surface modifications in the aged electrode enabled mechanistic pathways for byproduct formation while also enhancing the reaction kinetics for ammonia.



HRTEM images pristine (I) and aged (II) Co3O4. III illustrates NH3 catalytic performance (FE/YR).

Agradecimentos/Acknowledgments

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Study of electrochemical depolymerization of lignin in alkaline media on MnO2

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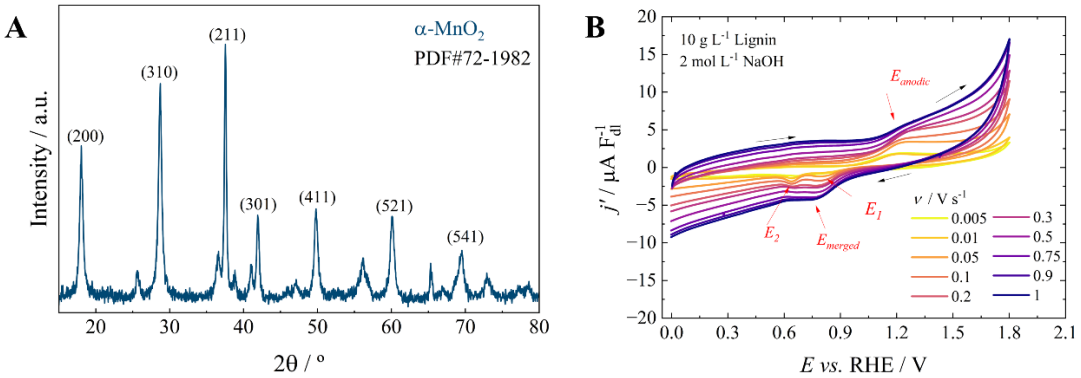
Palavras Chave:*Lignin depolymerization,Electrocatalysis,Reaction kinetics,Nanostructures,Monophenolic products*

Highlights

Pseudocapacitive adsorption behavior of intermediates on electrode; kinetics results suggest multistep electron transfer; lignin fragmentation into radical species; monophenolic products were found.

Resumo/Abstract

Fossil fuel, as primary energy source, undeniably resulted in the development of humanity over time; however, such growth resulted in a massively uncompensated rate of greenhouse gases emission. Scientific efforts have been focused on finding different ways to overcome this unbalanced rate. Alternatively, biorefinery presents a renewable and robust source to produce biofuel, chemical compounds, and rigid materials from lignocellulosic biomass. Yet, lignin's structural complexity hinders its selective depolymerization, challenging the transition to a cleaner process. Electrocatalysis can be used as feasible, and selective approach to depolymerize lignin instead. Thus, this work investigates the electrochemical depolymerization of eucalyptus Kraft lignin in alkaline media using MnO_2 as low-cost and versatile electrocatalyst. MnO_2 nanostructures were synthesized via hydrothermal method, and characterized by X-ray diffraction (XRD) using a Rigaku Smartlab (Cu-Kα: 1.54186 Å). For electrochemical tests, the material was drop-casted onto glassy carbon disk working electrode. Reference and auxiliary electrodes were a reversible hydrogen (encapsulated H_2 bubble around a Pt wire), and a graphite rod, respectively. Tests were performed using a potentiostat 302N Autolab. Before each lignin assay, MnO_2 film underwent voltametric cycling in 2 mol L^{-1} NaOH. Firstly, the nanostructures of MnO_2 were characterized by XRD, and the patterns, shown in Figure 1A, correspond to the diffraction of an α-phase, which is desired for electrocatalytic applications due to its tunnel structure. Figure 1B shows j-E potentiodynamic profiles in various scan rates for MnO_2 in 10 g L^{-1} lignin in 2 mol L^{-1} NaOH. Detailed analysis of these peaks revealed a pseudocapacitive adsorption for reaction intermediates, and a multistep electron transfer prior to the rate determining step. Moreover, products analysis after an oxidative stress at specific potentials confirmed the formation of monophenolic species.



A) XRD patters of MnO2 nanostructures; B) j-E potentiodynamic profiles at various scan rates.

Agradecimentos/Acknowledgments

FAPESP Grants #2019/22183–6, #2020/01177–5, #2025/02191-5, #2022/06405-1; RCGI/FAPESP Grant #2020/15230–5; CNPq Grants #306060/2017–5, #161023/2021–5, #311419/2023–2; CAPES Finance Code 001; and Shell Brasil (ANP) through the R&D levy regulation.

Surface Chemistry Engineering of Nanostructured Carbon Platforms for Electrochemical SERS Applications

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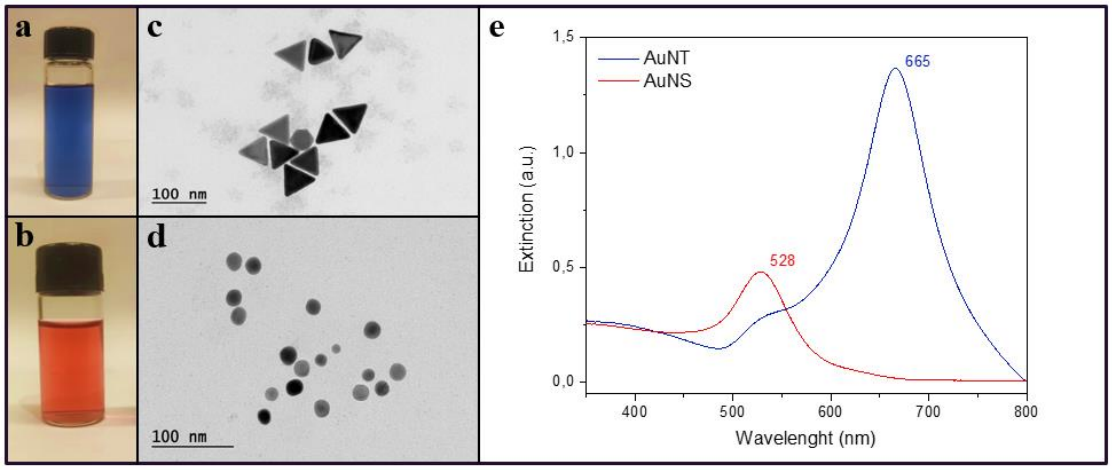
Palavras Chave:*Gold nanoparticles, vibrational spectroscopy, SERS effect, 4-NTP, carbon interfaces*

Highlights

Optimizing surface chemistry of carbon-gold nanostructures unlocks enhanced EC-SERS sensitivity for the detection of model analytes like 4-NTP, advancing bioelectronic sensing platforms.

Resumo/Abstract

The performance of nanostructured carbon platforms in electrochemical surface-enhanced Raman spectroscopy (EC-SERS) is strongly governed by the chemical nature of their surfaces. Precise adjustment of interfacial chemical environments enables control over molecular adsorption behavior and interfacial charge-transfer pathways, both of which are essential for achieving high sensitivity and signal reproducibility in SERS-based analyses. In this study, we explore strategies to modulate the surface chemistry of carbon nanostructures functionalized with gold nanoparticles with precisely controlled morphology, aiming to optimize their response in electrochemical SERS configurations. The investigation employs 4-nitrothiophenol (4-NTP) as a model molecular system due to its well-characterized interfacial and vibrational properties. The insights obtained from this approach provide a fundamental basis for the development of advanced EC-SERS platforms, with prospective applications in bioelectronic devices.



(a,b) AuNT and AuNS suspensions; (c,d) AuNT and AuNS TEM micrographs and e) extinction spectra

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Sustainable rGO/Manganese Oxide Thin Films: Electrochemical Activation and Application in Aqueous Pseudocapacitors

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Palavras Chave:*reduced graphene oxide,nanocomposites,electrochemical activation,aqueous pseudocapacitance,Manganese oxides*

Highlights

rGO/Mn oxide nanocomposites from manganese residue were processed as thin films and electrochemically activated, achieving 475 F $cm^{-3}$and 902 F g^{-1} in aqueous sodium pseudocapacitors.

Resumo/Abstract

The growing demand for energy storage drives the development of more sustainable electrodes and electrolytes. In this context, aqueous devices stand out due to their higher safety, lower environmental impact, and the use of abundant metals, such as sodium. Manganese is an attractive electrode material because it is non-toxic, abundant, low-cost, and suitable for reuse [1]. In this work, the manganese-rich residue from the Hummers method [2] was valorized to obtain nanocomposites based on reduced graphene oxide (rGO) and manganese oxides. Using a modified route, graphite oxide was not subjected to the final washing step, allowing the preservation of manganese. The reduction of graphene oxide was carried out at room temperature for 30 minutes using sodium borohydride, simultaneously promoting the reduction of GO to rGO and the in situ formation of manganese oxide nanostructures, while the reduction of GO in the absence of manganese was not observed under the same conditions. The methodology enabled control of the rGO/manganese oxide ratio and achieved manganese reuse rates of up to 99.6%. The nanocomposites were processed as thin films via the liquid–liquid interfacial route [3]. Characterization was performed using Raman spectroscopy, X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, thermogravimetric analysis, and in situ Raman spectroelectrochemistry. After electrochemical activation by cyclic voltammetry, a partial transformation of Mn_3O_4 into MnO_2 was observed, accompanied by morphological changes. The activated film exhibited a volumetric capacitance of 475 F cm^{-3} at 0.25 A $cm^{-3}$and a specific capacitance of 902 F g^{-1} at 0.50 A g^{-1}, demonstrating high potential for aqueous pseudocapacitors and sustainable energy storage.

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Agradecimentos/Acknowledgments

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Synthesis and characterization of thin film electrodes of copper complexes based on 4-[2-(4-Pyridinyl)ethenyl]benzoic acid.

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Palavras Chave:*Photoeletrochemistry,Energy Conversion,Coordination compounds,CO2 Reduction,Coordination Compounds,CO2 Conversion*

Highlights

Photoeletrochemical evaluation of extended conjugated copper complexes on conductive substrates for possible application as eletrocatalysts for CO_2 conversion.

Resumo/Abstract

The increasing of CO_2 concentration in our atmosphere, and the consequent climate change, motivated the studies for the development of technologies for CO_2 capture and utilization. Metal-Organic-Frameworks (MOF) structures based on copper and 4-[2-(4-Pyridinyl)ethenyl]benzoic acid (PVB) ligand exhibited promising results for applications in CO_2 capture. This project is investigating a possible application of high surface area, conjugated copper MOFs as an electrocatalyst for CO_2 reduction. First, a thin film of Cu-PVB complex was deposited on Fluorine-Doped-Tin-Oxide (FTO) using a layer-by-layer technique in a Spin-Coater, with alternating dispersed solutions of 0.01M KPVB and 0.01M $CuCl_2$ in methanol. This methodology produced almost transparent films and the resulting FTO|Cu-PVB showed an absorption band around 367nm. XRD measurements revealed that the FTO|Cu-PVB did not achieve detectable crystallinity. The electrochemical properties were evaluated in 0.5M $NaHCO_3$ aqueous solution using Pt as counter electrode and Ag/AgCl as reference electrode; the measurements were performed in ambient illumination (in the “dark”) and under 5mW.cm^{-2} of 375nm LED illumination. The Open-Circuit-Potential corresponded to 0.27 mV in the dark and 0.14 under illumination. Cyclic voltammetry, performed at 10 mV s^{-1} from -0.1 V to 0.6 V (vs Ag/AgCl) revealed a capacitive current limited by hydrogen and oxygen evolution reactions (HER, OER). Higher current values were observed under irradiation; at 0.6 V, the current values corresponded to 0.03 µA.cm^{-2} in the dark and 0.12µA.cm^{-2} under irradiation; thus, the FTO|Cu-PVB exhibited the behavior of an n-type semiconductor. The Cu-PVB deposition is undergoing development as it enables better water stability, surface area and conductivity of the conjugated structures by achieving a more crystalline film and a more connected interface between the Cu-PVB and the FTO or semiconductor substrates such as some photoactive materials.

Agradecimentos/Acknowledgments

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Time-resolved electrochemical impedance analysis as a probing tool for finding electrocatalyst's active sites

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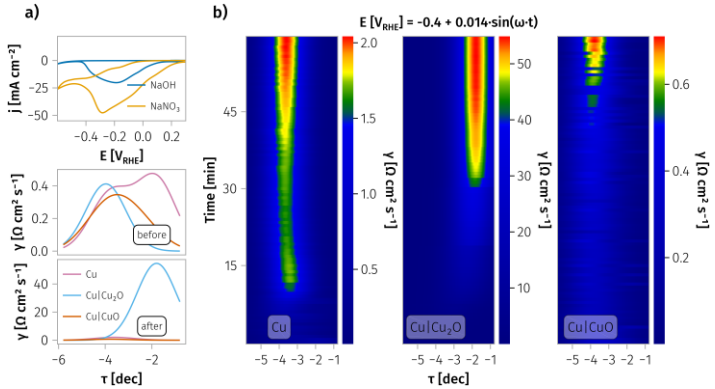
Palavras Chave:*EIS,DRT,NO3RR,Cu,CuOx*

Highlights

Operando DRT (model-free EIS) resolves interfacial kinetics for NO_3RR. Cu|CuO outperforms Cu and Cu|Cu_2O, showing faster charge-transfer and reduced impedance.

Resumo/Abstract

Evaluating catalytic active sites remains a central challenge in electrochemistry, as heterogeneous activity often emerges from a combination of exposed crystallographic planes, surface/edge defects, and morphology. Electrochemical impedance spectroscopy (EIS) is a powerful approach to probe interfacial polarization processes at the electrode surface. However, interpreting EIS typically relies on selecting an electrochemical model (*e.g.*, equivalent circuits). The distribution of relaxation times (DRT) offers a model-free alternative by deconvoluting impedance contributions according to their characteristic time scales. Under*operando*conditions, tracking how these time constants (τ) evolve can reveal whether a dynamically formed interface is catalytically relevant. Particularly, changes in the charge-transfer time scale may provide a direct indicator of interfacial activity. Here, DRT was employed to evaluate different Cu|CuO_x interfaces for nitrate reduction (NO_3RR). While pure Cu and CuO_x phases are often reported to show limited selectivity, literature indicates that reducing CuO_x to metallic Cu can yield near-unity Faradaic efficiency for NH_3. But which interface to choose from? To answer this, Cu foils were pre-passivated, by CA, to form either Cu_2O or CuO in NaOH pH 14, and further tested for NO_3RR. The corresponding Cu foil's CV is shown on Figure 1a.*Operando*DRT was collected throughout NO_3RR (Figure 1b). The Cu|CuO interface exhibited accelerated charge-transfer kinetics upon NO_3^- addition (lower τ) and less resistance (intensity γ) values, whereas Cu|Cu_2O revealed a rate determining adsorption-like process around 10^{-2} s. Beyond identifying the most active interface, this framework can be integrated with; i)*in situ*structural probes (*e.g.*, Raman and XAS); ii)*online*molecular characterizations (DEMS and FTIR) and iii) long-duration operation, enabling Faradaic efficiency, yield rate and overpotential to be correlated with DRT-resolved processes.



a) CV and b) operando DRT of Cu, Cu|CuO and Cu|Cu2O for NO3RR.

Agradecimentos/Acknowledgments

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Zn-Co coatings from ethaline as corrosion inhibitors

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Palavras Chave:*Electrodeposition,Deep eutectic solvents,Ethaline*

Highlights

ZnCo coatings were electrodeposited from ethaline. ZnCo coatings showed excellent corrosion resistance, evidenced by the increased capacitive arc. Co addition increased the nobility of the coatings.

Resumo/Abstract

The search for more sustainable routes to obtain these surfaces has driven the use of ethaline, a solvent formed by combining choline chloride and ethylene glycol (1ChCl:2EG), named deep eutectic solvents (DES), is notable for its biodegradability, good ionic conductivity, and low relative cost. The objective of this work was to obtain Zn-Co films in ethaline on 1020 carbon steel discs. For this, $[Zn^{2+}]$:$[Co^{2+}]$ was used in proportions 16:1 and 1:16. In the electrochemical tests, a conventional three-electrode electrochemical cell was used. The working electrode was a 1020 steel disc, the reference electrode was Ag/AgCl/DES, and the auxiliary electrode was a Pt plate. The reduction potentials −1.3 V and −1.0 V for Zn^{2+} and Co^{2+}, respectively, were obtained by cyclic voltammetry at 70 °C. The most negative potential for electrodeposition and the theoretical thickness of 1 µm were chosen. The morphology of the Co-rich coatings (Co and Zn_3Co_{97}) showed cracks. When analysing those that contained mostly Zn (Zn and $Zn_{96}Co_4$), the morphology changed from non-uniform crystallites to a more uniform, homogeneous layer. In the corrosion tests, linear potentiodynamic polarization (PPL) and electrochemical impedance spectroscopy (EIE) were used in 0.1 mol L^{-1} NaCl. After 1 hour of immersion, the open-circuit potentials were −0.55 V, −0.98 V, and −1.02 V for coatings rich in Co, Zn, and $Zn_{96}Co_4$, respectively, results like those obtained by PPL. This indicates that adding Co to the coating made it more noble. The EIE results indicated that incorporating Co increased corrosion resistance, as evidenced by the increase in the capacitive arc. The influence of immersion time for $Zn_{96}Co_4$ was also evaluated. Within 2 h in the presence of 0.1 mol L^{-1} NaCl, there was no significant change; For 3 h and 4 h, a significant reduction in the capacitive arc was observed in the Nyquist diagrams, indicating the possible fragility of the coating, most likely due to the reduced thickness.

Agradecimentos/Acknowledgments

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49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

FIS - Físico-Química

A Clustering Algorithm Coupled with DFT for the Design of Highly Selective MIPs for Profenofos

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Palavras Chave:*DFT,MIP,Algorithm,Pesticides,Simulation*

Highlights

A DFT-based approach combined with a proprietary clustering algorithm was used to screen candidate FM/SM systems for profenofos-targeted MIPs and assess selectivity against six potential interferents

Resumo/Abstract

Molecularly Imprinted Polymers (MIPs) are highly selective recognition elements for sensing, and their performance depends strongly on the choice of template, functional monomer (FM), structural monomer (SM), and solvent [1–3]. In the noncovalent imprinting approach, analyte–FM complexes formed in the pre-polymerization mixture direct the formation of complementary binding cavities after polymerization and template removal [4-6]. To focus the experimental effort, we combined Density Functional Theory (DFT) with an original algorithm developed by our group, the Molecular Binding Algorithm by Surface Mapping (MBASM) [7], to screen candidate FM/SM systems for a profenofos-targeted MIP and assess selectivity against six potential interferents. 32 monomers were evaluated: for each analyte–monomer pair, MBASM generated 40 initial complexes (8960 total across seven analytes). All geometries were optimized in gas phase at the B3PW/def2-SVP level using ORCA software; frequency calculations were perfomed to confrmed that each of the isolated molecules were at mininma of the potential energy. The lowest-energy complexes were then re-optimized at B3PW/def2-TZVP level theory and used for solvent screening in acetonitrile, chloroform, ethanol, methanol, and water with the SMD model. All calculations employed RIJCOSX and included the geometric counterpoise correction for triple-z basis sets. Preliminary results indicate 1,4-Divinylbenzene (DVB), -0.57 eV, as the most suitable SM because it consistently exhibits weaker binding, minimizing competition with analyte–FM interactions, while p-amino benzoic acid (PABA), -0.81 eV, emerges as the most promising FM for profenofos selectivity. As an experimental guideline, malathion, dichlorvos, and acetamiprid, soluble in the same synthesis medium as profenofos, were prioritized as the most stringent interferents, while additional interferents will be tested in alternative solvents where profenofos has low solubility.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP (Grant No. #2024/12623-7) and the Institute of Chemistry (IQ–USP), University of São Paulo.

Activated carbon from Capsicum baccatum waste for tetracycline adsorption.

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Palavras Chave:*Emerging pollutants, tetracyclines, Capsicum baccatum, activated carbon, adsorption.*

Highlights

Emerging pollutants persist in the environment; tetracyclines are mostly unmetabolized; Capsicum baccatum biomass produces activated carbon with suitable properties for its adsorption.

Resumo/Abstract

Emerging pollutants comprise substances whose environmental presence and effects were previously undocumented, including pharmaceuticals, personal care products, pesticides, and microplastics. These contaminants originate from diverse anthropogenic activities and enter natural systems through multiple pathways, promoting bioaccumulation along trophic chains and inducing biochemical disturbances in exposed organisms. Among them, tetracyclines stand out as a widely used class of antibiotics composed of an octahydrotetracene-2-carboxamide core with substituents that determine their physicochemical behavior, with key reactions occurring on the C and D rings. Owing to limited metabolic transformation—only about 20% is metabolized in humans and animals—large fractions are excreted unmetabolized, contributing to environmental dissemination. Activated carbons (AC), derived from a broad range of carbonaceous precursors, exhibit structural and chemical features that enable efficient interactions with adsorbates through physisorption and chemisorption. Among potential precursors, the pimenta dedo-de-moça (Capsicum baccatum) is abundant in South America and widely used in culinary applications. Its biomass shows favorable characteristics for AC production, with proximate analysis indicating high volatile content (73.55%), low ash content (4.51%), and suitable fixed carbon (21.93%). Aromatic constituents promote graphitic domain formation, while nitrogen-containing alkaloids enhance surface functionalization, improving adsorption performance. The AC presented SBET, pore volume, and average pore diameter of 2827 m^2/g, 1.49 cm^3/g, and 2.12 nm, respectively, as determined by N_2 physisorption. SEM images (Scios Dual Beam) confirmed the development and expansion of pore structures after activation, supporting its applicability in adsorption-based remediation.

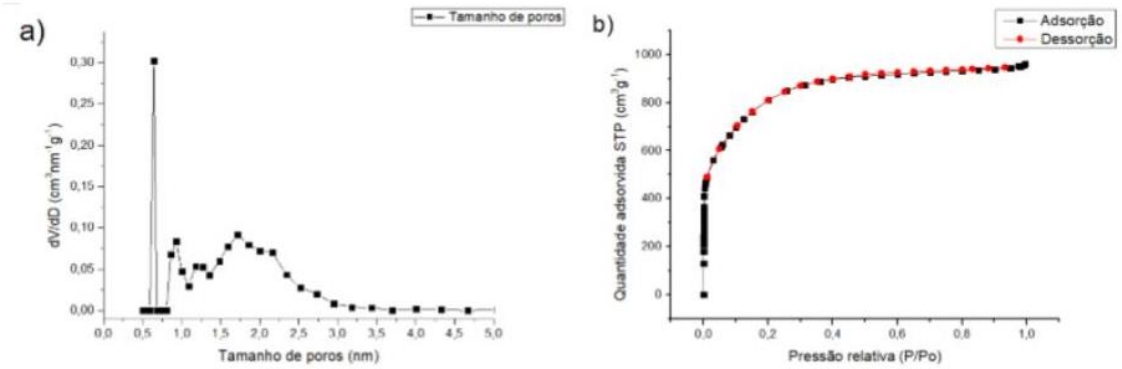


Fig. a) pore size distribution; b) N_2 adsorption–desorption isotherms.

Agradecimentos/Acknowledgments

I express my gratitude to the Universidade Estadual de Maringá (UEM), COMCAP-UEM, Grupo de Materiais Carbonáceos Multifuncionais (GMCM) and CAPES for their financial support and for providing the infrastructure for the development of this research.

Adsorption of Copper (II) onto porous carbonaceous material derived from brewery waste: kinetic study and response surface optimization

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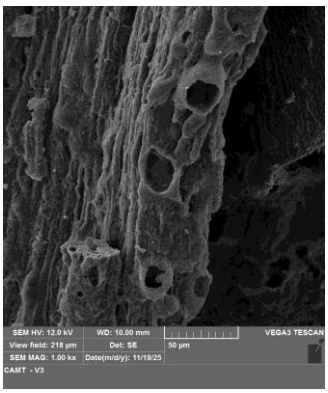
Palavras Chave:*copper (II),adsorption,carbonaceous material,RSM,kinetics*

Highlights

Carbonization of brewery residue produced a porous material. Kinetic and equilibrium models evaluated adsorption. RSM increased Cu(II) removal from 14% to over 30%.

Resumo/Abstract

Industrial activity generates significant environmental impacts, mainly due to the improper disposal of waste, making the development of efficient wastewater treatment technologies indispensable. Among these technologies, adsorption stands out in the removal of toxic metals, such as copper (II), widely present in industrial effluents, pesticides, and electronic waste. In this context, carbonaceous materials obtained from residual biomass have attracted interest for combining high adsorptive efficiency with waste valorization. In this work, the adsorption of Cu^{2+} was investigated using a carbonaceous material produced by the carbonization of brewery waste, with chemical activation by KOH. The kinetics and equilibrium of the process were evaluated, as well as the influence of pH, initial metal concentration, and adsorbent mass, using Response Surface Methodology. The biomass and carbonaceous material were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). Textural properties were determined by N_2 adsorption/desorption isotherms. The results indicated that the material has adequate porosity for the adsorption process, with micro- and mesopores, a specific surface area of 251.62 $m^2\ g^{-1}$, and a total pore volume of 0.17 $cm^3\ g^{-1}$. XRD diffractograms showed aromatic and graphitic carbonaceous structures, while FTIR spectra showed bands typical of lignocellulosic materials, with changes after activation. The kinetics were best described by the pseudo-first-order model (R^2 = 0.74), suggesting a predominance of physisorption. The DCCR design (17 trials) indicated pH and initial Cu^{2+} concentration as the most significant variables, with lower pH and lower initial concentrations favoring removal. It is concluded that carbonaceous material obtained from brewery waste has potential for the removal of trace metals from wastewater.



Micrografia do material carbonáceo produzido a partir do resíduo cervejeiro

Agradecimentos/Acknowledgments

The authors thank the Federal University of Bahia and the University of Salvador for infrastructure support, and CAPES, FAPESB, and the Graduate Program in Chemical Engineering for doctoral and undergraduate scholarships.

A Geometry-Informed Cutoff for Many-Body Electrostatics

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Palavras Chave:*electrostatics,polarization,many-body,bispherical,cutoff*

Highlights

Dielectric polarization makes electrostatic interactions inherently nonadditive; Many-body BIE efficiently resolves them; A geometric parameter enables a cutoff with bounded error.

Resumo/Abstract

Electrostatic interactions govern diverse natural and engineered particulate systems, including dust and aerosols, cloud microphysics, and soft-matter assemblies such as colloidal aggregates and self-assembled materials. In many cases, the particles are dielectric, making electrostatics intrinsically nonadditive: the induced surface charge on any particle is set by the total electric field, which itself includes contributions from induced charges on all other particles. An accurate and efficient boundary-integral equation (BIE) formulation has been established for many-body dielectric electrostatics, making explicit how geometry and dielectric contrast regulate mutual polarization. [E. B. Lindgren et al., J. Comput. Phys. 371 (2018) 712-731; E. B. Lindgren, J. Chem. Theory Comput. 21 (2025) 6135-6150] With sufficient size or charge asymmetry, naive Coulombic expectations may be overturned, enabling like-charge attraction and force contributions from nominally neutral particles, with local fields far exceeding monopole estimates. To make computations scalable, a geometry-informed cutoff selectively neglects mutual polarization between sufficiently separated pairs while retaining the full monopole contribution of free charge. Truncation is determined by a dimensionless geometric parameter, s*, derived from bispherical coordinates: pair couplings exceeding an s*-based threshold are neglected, reducing computational cost while keeping errors controlled. The error behaves nonmonotonically as the cutoff is tightened, consistent with partial cancellation among many-body contributions. The cutoff is not merely practical: s* controls exponential attenuation of inter-particle multipole coupling, bounding truncation error and quantifying the strength of neglected polarization.



Cutoff is controlled by local geometry. Reference spheres: black; retained couplings: medium gray.

A Low-Cost Machine Learning Fine-Tuning Approach for Adsorption Energy Prediction

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Palavras Chave:*Machine learning,electro-oxidation,computational chemistry*

Highlights

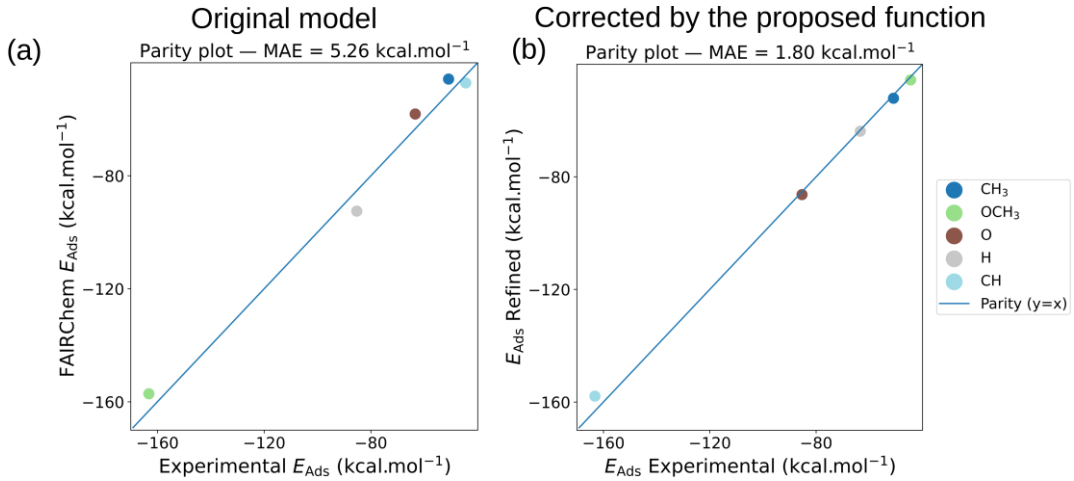
The fine-tuning of a machine learning model with synthetic data built using a permutationally invariant correction and experimental data yields a cost-effective approach to accurate adsorption energy

Resumo/Abstract

Accurate adsorption energies (EAd_s)for methanol electro-oxidation (MEOR) intermediates on platinum are essential for catalyst design [1]. Machine learning models, such as the Universal Model for Atoms (UMA), offer density functional theory (DFT) level accuracy at a reduced computational effort. However, achieving chemical accuracy remains critical for reliable kinetic and mechanistic predictions [2]. In this work, the pre-trained “uma-s-1p1” model was applied to predict the adsorption energies of adsorbates representative of MEOR intermediates (OCH_3, CH, CH_3, H and O) on Pt(111), and subsequently fine-tuned by using a permutationally invariant correction function proposed in this work. The parity plot of the “uma-s-1p1” and experimentalEAd_svalues [3], are shown in Figure 1a. To improve the energetic description, a fine-tuning database was constructed from potential energy curves and molecular dynamics trajectories for each adsorbate, corrected for both energies and forces using the proposed function. The refined trajectories were then used to fine-tune the “uma-s-1p1” model, excluding CH to assess possible overfitting. As shown in Figure 1b, the MAE is reduced from 5.26 to 1.80 kcal mol^{-1} after the finetuning procedure with the proposed function. The slight improvement observed for CH confirms that the refinement does not induce overfitting and preserves model transferability. The proposed permutationally invariant correction thus provides an efficient and physically consistent strategy to achieve chemically accurateEAd_svalues.

References

[1] Zhang et al. Chem. Rev. 122 (2022), [2] Ramakrishnan, R, et al. J. Chem. Theo. Comp. 11 (2015) [3] Wellendor et al. Surf. Sci. 640 (2015).



Parity plots of the experimental EAds and the calculated by: (a) uma-s-1p1, (b) refined model

Agradecimentos/Acknowledgments

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Alumina mesoporosa obtida utilizando CTAB e tartarato como co-templates – ordenamento da estrutura e relação com a atividade catalítca

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Palavras Chave:*Alumina mesoporosa ordenada, Co/Al2O3, CTAB, tartarato, decomposição catalítica de etanol*

Highlights

Mesoporous alumina synthesized via CTAB-tartrate cooperative assembly; Co/Al2O3 catalysts tested for ethanol decomposition; Ordered mesoporous alumina structures favored carbon nanotube formation

Resumo/Abstract

Foram preparados catalisadores de cobalto suportados em alumina mesoporosa (Co/Al2O3), que foram testados na reação de decomposição catalítica do etanol. A síntese da alumina foi realizada via rota hidrotérmica, utilizando sulfato de alumínio como precursor, uréia como agente precipitante e o sistema CTAB/tartarato de sódio como direcionadores de estrutura. A adição controlada do tartarato (hidróxi-carboxilato) atuou como ponte de interação entre as espécies de alumínio e as micelas do surfactante catiônico, permitindo a modulação da porosidade. Variou-se a proporção entre tartarato/Al para verificar o efeito no grau de ordenação estrutural. Após a calcinação da amostra, com formação de alumina, a fase ativa (Co) foi incorporada pelo método de impregnação, com teor de Co de 10% em massa. Os materiais foram caracterizados por análise termogravimétrica, adsorção-dessorção de N2, espectroscopia Raman, microscopia eletrônica de varredura (MEV) e SAXS (Small Angle X-Ray Scattering). As análises de SAXS revelaram quais foram as amostras de alumina com maior ordenamento de mesoporos Os testes catalíticos de decomposição do etanol revelaram uma forte correlação entre o grau de ordenamento da alumina e o rendimento em carbono, que estava na forma de nanotubos. Observou-se que suportes com estrutura mesoporosa ordenada e elevada área superficial (obtidos com maior razão tartarato/Al) favoreceram significativamente a formação de carbono. Em contrapartida, suportes desordenados apresentaram menor atividade para a deposição de carbono. Os resultados sugerem que a arquitetura regular dos poros da alumina mesoporosa é crucial para a dispersão adequada das partículas de cobalto, prevenindo a sinterização excessiva e potencializando o crescimento de nanoestruturas de carbono.

Agradecimentos/Acknowledgments

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E agradeço aos meus amigos na faculdade

Análise Computacional da Estereosseletividade de Rearranjos de Johnson-Claisen em Cicloenonas

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Palavras Chave:*DFT,TS,Estereosseletividade,Princípio de Curtin-Hammett,Rearranjo de John-Claisen,REarranjo de Johnson-Claisen,Curtin-Hammett*

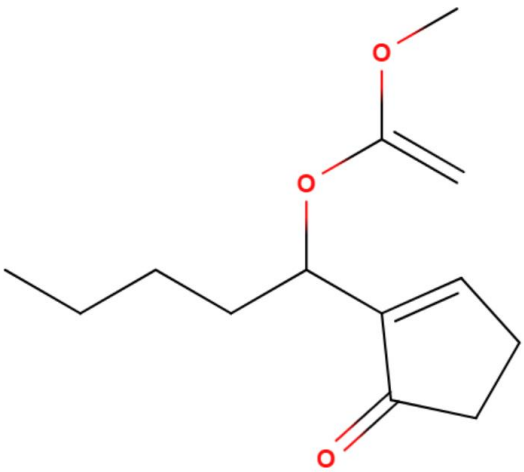
Highlights

DFT study of stereoselectivity in the [3,3]-sigmatropic rearrangement of a cycloenone-derived allyl enol ether.

Benchmarking (M06-2X, ωB97X-D and B3LYP) showed consistency with experimental data.

Resumo/Abstract

Os rearranjos de Claisen, poderosas ferramentas sintéticas, são especialmente utilizados devido à economia de átomos e ao controle termodinâmico que proporcionam. Este trabalho buscou investigar a esterosseletividade do rearranjo de Johnson-Claisen de um éter alílico do enol de uma cicloenona, por meio de cálculos quânticos utilizando a Teoria de Funcional de Densidade (DFT). A DFT é uma metodologia amplamente reconhecida para a elucidação de estruturas moleculares, propriedades eletrônicas e caminhos de reação de moléculas orgânicas, além de auxiliar na obtenção de informações termodinâmicas. De acordo com a literatura, não existe um funcional universalmente adequado para cálculos de estados de transição, sendo necessário um estudo de benchmarking de alguns funcionais (M06-2X, ωB97X-D e B3LYP) para o estudo de sistemas cíclicos. Para os cálculos das propriedades termoquímicas da molécula foi aplicado o princípio de Curtin-Hammett para estimar a razão E/Z dos produtos. Ademais, foi realizada uma correção térmica quasi-harmônica nos resultados, a uma temperatura de 383,15 K, utilizando o programa GoodVibes. Os resultados mostraram que as proporções estereoisoméricas obtidas teoricamente, com e sem correção térmica, ficaram muito próximas do valor experimental obtido por Chapuis e colaboradores [1]. Por fim, os resultados teóricos foram consistentes com os dados experimentais, indicando o potencial do modelo utilizado. A correção térmica alterou os valores da razão E/Z, porém sem variações significativas. [1] Chapuis, C., Büchi, G. and Wüest, H. (2005), Synthesis of*cis-Hedione*® and Methyl Jasmonate*via*Cascade*Baylis–Hillman*Reaction and*Claisen*Ortho Ester Rearrangement. HCA, 88: 3069-3088.



Molécula analisada neste estudo

Agradecimentos/Acknowledgments

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Análise conformacional e caracterização eletrônica da bixina

Isaac Oliveira Miranda Magalhães (IC)*[1], Leonardo Carneiro Toscano de Oliveira (PQ)[1], Luana Lemos Reis (PQ)[1], Pierre Carlos de Souza Junior (PQ)[1], Daniel Francisco Scalabrini Machado (IC)[1], Ricardo Gargano (PG)[1], João Batista Lopes Martins (PG)[1].

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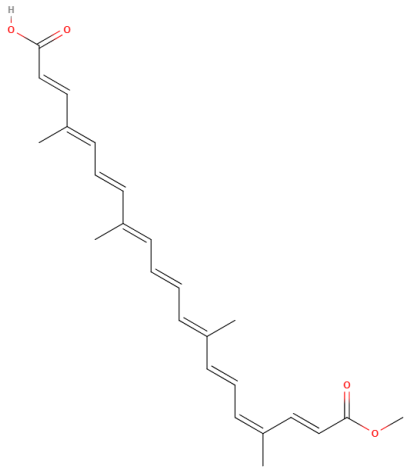
Palavras Chave:*Caratenóide Natural Bixina, Métodos DFT e TD-DFT, Conformação Molecular, Propriedades Óticas, Células Solares.*

Highlights

Computational study of Bixin as a dye for DSSCs, refining UV-Vis spectra via TD-DFT and conformational analysis to bridge the gap between theory and experiment.

Resumo/Abstract

Este estudo é um estudo teórico-computacional sobre a bixina, um carotenóide natural extraído do urucum com grande potencial para células solares sensibilizadas por corantes (DSSCs). O objetivo central é estabelecer um protocolo computacional que correlacione a estrutura conformacional da molécula com suas propriedades ópticas, buscando superar as discrepâncias comuns entre espectros teóricos e experimentais. Inicialmente, realizou-se uma busca conformacional sistemática com o código CREST, utilizando o método semiempírico GFN2-xTB. Foram identificados entre 120 e 160 confórmeros dependendo do solvente (clorofórmio, metanol ou DMSO). As dez conformações mais estáveis foram selecionadas para análises detalhadas. Em seguida, as propriedades eletrônicas e de absorção foram calculadas via Teoria do Funcional da Densidade (DFT) e sua extensão dependente do tempo (TD-DFT) no software Gaussian16, empregando funcionais híbridos como B3LYP-D3, CAM-B3LYP-D3 e wB97XD, combinados a diferentes conjuntos de base. Os resultados preliminares revelaram um desvio batocrômico sistemático de aproximadamente 100 nm quando se utiliza apenas o método GFN2-xTB para a previsão espectral. A análise detalhada indicou que essa divergência não provém de grandes distorções geométricas, mas de variações sutis no parâmetro de Alternância de Comprimento de Ligação (BLA), que modula o gap de energia. Além disso, observou-se que o modelo de solvatação implícita apresenta limitações em solventes próticos como o metanol, onde interações específicas de ponte de hidrogênio e efeitos de agregação podem influenciar o deslocamento do pico de máxima absorção.
Em conclusão, o estudo valida a necessidade de re-otimização via DFT para obter precisão espectral. Os protocolos estabelecidos servirão de base para o desenho racional de novos corantes e para a criação de bancos de dados voltados ao treinamento de modelos de machine learning na predição de propriedades fotovoltaicas.



Estrutura 2D da cis-bixina

Agradecimentos/Acknowledgments

CNPq, Fap-DF, Capes, UnB, LMSC, LQC, LEEDMOL

Análise Paramétrica das Isotermas de Adsorção BET (Tipos I–V): Interpretação Física, Comportamento Matemático e Aplicações

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Palavras Chave:*Mecanismo de adsorção, parâmetros físicos de isotermas, condições de contorno das isotermas de adsorção, aprimoramento tecnológico, aplicabilidade industrial e socioambiental*

Highlights

All five BET categories are linked to distinct adsorption mechanisms and surface morphologies.A parametric analysis of BET I-V isotherms reveals how Nm, n and $C_1/_2$ control adsorption curve morphology.

Resumo/Abstract

Estudos sobre processos de adsorção são fundamentais para o desenvolvimento de materiais aplicados ao tratamento de águas, efluentes, catálise e indústria farmacêutica. A compreensão dos mecanismos permite a proposição de tecnologias e soluções para desafios ambientais e industriais. Nesse contexto, este trabalho investiga o comportamento físico e matemático das isotermas de adsorção do tipo Brunauer, Emmett e Teller (BET). As isotermas descrevem a relação entre a quantidade adsorvida(Qe) e a concentração do adsorvato no equilíbrio (Ce), sendo influenciadas pela porosidade e natureza dos sítios ativos do adsorvente e a intensidade das interações adsorvato–adsorvente. As isotermas BET são classificadas em cinco tipos (I–V), que diferem quanto à morfologia e ao mecanismo de adsorção. As isotermas do tipo I representam materiais microporosos, com rápida saturação em baixas concentrações. As do tipo II descrevem superfícies não porosas ou macroporosas, com formação progressiva de monocamadas e multicamadas. O tipo III ocorre em sistemas de baixa afinidade, sem formação definida de monocamada. As isotermas do tipo IV são típicas de materiais mesoporosos, com condensação capilar e platô de saturação. Já o tipo V apresenta comportamento cooperativo, com baixa adsorção inicial seguida de aumento acentuado. Em todas as isotermas, três parâmetros são comuns: a capacidade adsortiva máxima de monocamada (Nm), o número de camadas (n) e a concentração correspondente à metade da saturação ($C_1/_2$). Neste estudo, os modelos foram analisados fixando-se os parâmetros e variando-se apenas um deles, permitindo identificar os intervalos de variação que preservam a morfologia das curvas e elucidar o significado físico de cada parâmetro. Conclui-se que a análise paramétrica das isotermas BET é uma ferramenta poderosa para interpretar mecanismos de adsorção, prever comportamentos experimentais e orientar a seleção de materiais para aplicações tecnológicas.

Analysis of photocatalytic potential of heterostructures based on sodium-potassium niobate with reduced graphene oxide

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Palavras Chave:*Heterostructure,sodium potassium niobate,graphene oxide,photocatalysis.*

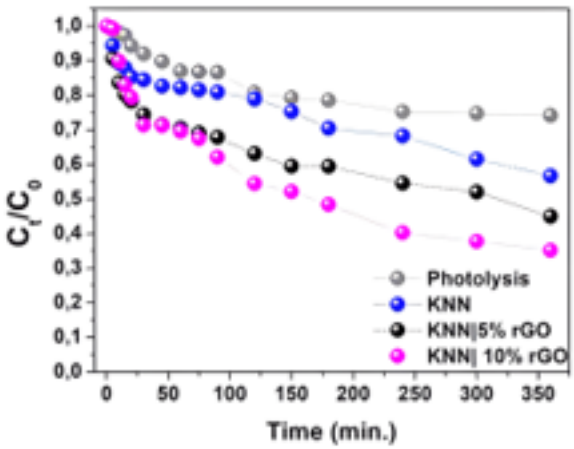
Highlights

Heterostructure based on $K_{0.5}Na_{0.5}NbO_3$ with reduced graphene oxide showed promising photocatalytic activity using Rhodamine 6G.

KNN/xrGO (x = 5, 10% m/m) heterostructure exhibited the best performed.

Resumo/Abstract

Potassium-sodium niobate ($K_{0.5}Na_{0.5}NbO_3$ -KNN) is a remarkable lead-free ferroelectric material, making it an essential candidate in the quest for sustainable and high-performance electronic applications. Hovewer, alkalin niobates are characterized by a large band gap of approximately 3.2 eV, which limits their application in photocatalysis. Modifications such as doping and incorporation into heterostructures containing semiconductors and/or carbon-based materials show promise for enhancing the photocatalytic activity of these materials, both in terms of band structure and surface area. In this sense, this work aimed at the synthesis, structural characterization and evaluation of photocatalitc potential of heterostructures of KNN with reduced graphene oxide (rGO), KNN/xrGO (where x = 5, 10% m/m). KNN was prepared by ultrasonic spray pyrolysis and the graphene oxide by the Hummers method. The heteroestructure KNN/xrGO was obtained by impregnation method. The charcaterization of the heterostrucutes were performed by XRD, FTIR, SEM, and UV-Vis (DRS). The photocatalytic potential was investigated using Rhodamine 6G as a test molecule. Structural and morphological characterizations confirmed the formation of heterostructures exhibiting characteristics of both KNN and rGO. The analysis of the photocatalytic potential showed degradation rates of 68% and 80% for the KNN/5% rGO and KNN/10% rGO heterostructures, respectively, representing improvements of up to 20% compared to pure KNN and to the dye degradation in the absence of photocatalysts. The reaction kinetics were up to 1.5 times higher for the heterostructure containing 10% rGO. The results demonstrated that the proposed systems were successfully developed, with improved photocatalytic activity resulting from heterostructure formation.



Kinetics of Rhodamine 6G dye degradation in the absence and in the presence of photocatalysts.

Agradecimentos/Acknowledgments

FAPESP, CNPq, CAPES, PIBIC - UNESP

Analysis of the Electrocatalytic Performance of Polypyrrole-Functionalized Sensors for Glucose Detection

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Palavras Chave:*chronoamperometry,cyclic voltammetry,polymer,low-cost,biosensor*

Highlights

Cyclic voltammetry and chronoamperometry measurements are used to analyze the electrocatalytic performance of polymer-functionalized gold electrodes for glucose detection.

Resumo/Abstract

Biosensors are compact and cost-effective devices that utilize biological recognition to identify diseases and facilitate diagnoses.1 Multidisciplinary advances in biology, electronics, and materials research have made it possible to apply biosensors in different contexts, such as continuous monitoring, leading to rapid results and minimally invasive testing.2 Biosensors can vary in the recognition units used, including enzymes, antibodies, microorganisms, and nucleic acids.3 Here, gold-electrode sensors functionalized with the conductive polymer polypyrrole (PPy) are employed for glucose detection, being evaluated at different analyte concentrations (Figure 1). PPy electrodeposition on the gold electrodes is performed using chronoamperometry. Chronoamperometry and cyclic voltammetry data were collected using the prepared electrodes and subsequently analyzed with Python, allowing for the generation of various calibration curves from the results. Our preliminary findings indicate that the sensitivity of the PPy-functionalized electrode to glucose under the tested conditions is up to six times higher than that of the non-functionalized electrodes (i.e., 43.3 ± 2.3 and 7.6 ± 2.2 μA/decade, respectively). The subsequent experiments include (i) the use of complementary glucose concentrations to evaluate sensors' limit of detection, and (ii) the glucose oxidase (GOx) enzyme immobilization at the electrode surfaces. In addition to enhancing specificity, the incorporation of GOx seeks to improve the sensitivity of the PPy-functionalized electrode through porous activation. The combination of high-quality, porous PPy electrodes with GOx offers a promising avenue for real-time biosensing, setting the stage for the development of more convenient diagnosis tools.

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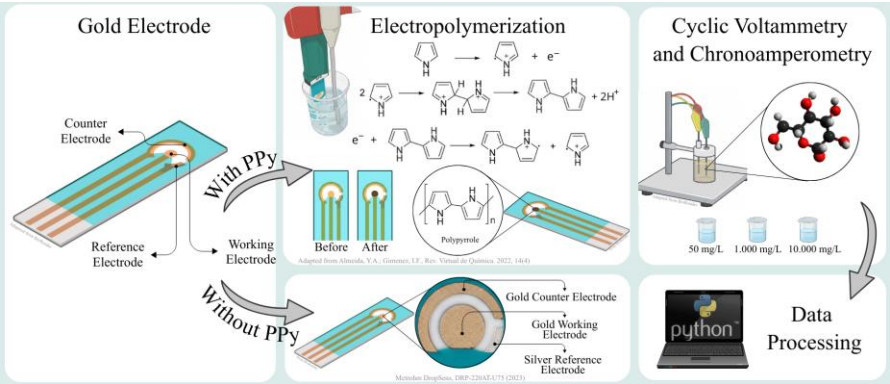


Figure 1 – Schematic diagram of the project development stages.

Agradecimentos/Acknowledgments

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Antimicrobial and Hemocompatible surface coatings based on PDMAEMA/heparin polyelectrolyte multilayers containing ionic liquids

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Palavras Chave:*Layer-by-Layer Multilayers, Polyacrylates, Polymers, Anticoagulant*

Highlights

Long-chain ionic liquids altered the surface properties and reduced bacterial adhesion. The ionic liquids on the surfaces delayed the whole-blood coagulation.

Resumo/Abstract

Medical device–associated infections and thrombosis continue to pose significant challenges, driven by bacterial infections and undesirable blood–material interface interactions. In this work, we expand the application of multifunctional polyelectrolyte multilayer (PEM) coatings containing ionic liquids (ILs). These coatings were fabricated on plasma-pretreated polystyrene substrates (PS) using a layer-by-layer approach. PEMs based on poly[(2-dimethylamino)ethyl methacrylate] (PDMAEMA) and heparin (HP), incorporating long-alkyl-chain ILs, were prepared. The concentration of ILs embedded in the PEMs was adjusted, as in previous work, to achieve cytocompatibility. The formation and stability of the PEMs were confirmed by wettability measurements, atomic force microscopy, and X-ray photoelectron spectroscopy. PEMs composed of PDMAEMA and HP without ILs supported bacterial adhesion and proliferation. In contrast, the presence of ILs in the PEMs led to changes in surface reorganization and nanomechanical behavior, resulting in reduced adhesion energy and enhanced antimicrobial activity against*P. aeruginosa*and*S. aureus*. The PEMs with ILs imparted reduced platelet recruitment compared to the PDMAEMA/HP PEM and PS. The surface coverage decreased from 19.2% on pristine PS to 7.5% on PDMAEMA/HP PEMs and to approximately 4.0% when ILs were incorporated. A similar trend was observed for leukocyte adhesion, which decreased from 21.0% on PS to 1.7% on PDMAEMA/HP PEM and to around 0.5% on PEMs embedded with ILs. Whole-blood clotting kinetics revealed a pronounced delay in blood clot formation on PEM-coated surfaces, primarily on those containing ILs for up to 60 min. Stability tests in phosphate-buffered saline further indicated partial surface reorganization of IL-containing PEMs while preserving their interfacial functionality. These results reveal that PDMAEMA/HP PEMs incorporating adjusted amounts of ILs provide an effective strategy for engineering polymeric interfaces.

Agradecimentos/Acknowledgments

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Application of polymeric monoliths based on cellulose acetate/cellulose acetate butyrate for bisphenol A adsorption in aqueous medium

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Palavras Chave:*Polymeric monoliths, Cellulose acetate, Adsorption, Bisphenol A, Emerging pollutants*

Highlights

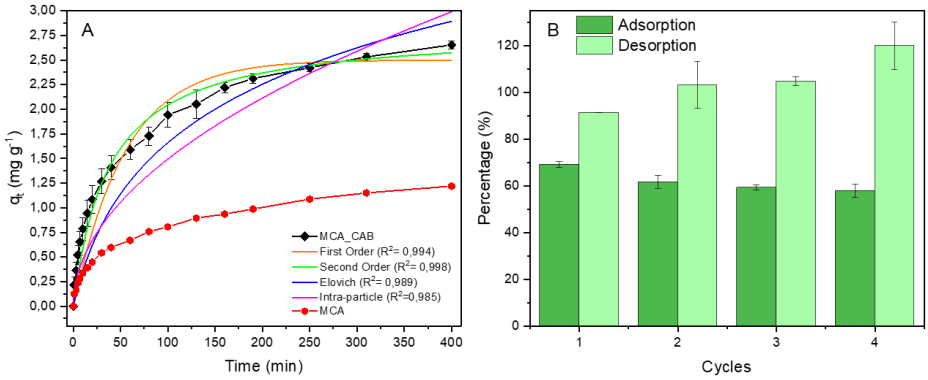
Cellulose acetate (CA)/cellulose acetate butyrate monolith doubled the adsorption capacity of Bisphenol A (2.6 mg/g) compared to the CA monolith, maintaining stability over four reuse cycles.

Resumo/Abstract

Bisphenol A (BPA) is a synthetic compound whose migration into aqueous media represents an environmental and human health risk due to its endocrine-disrupting activity[1]. In this context, cellulose-derived polymeric monoliths have stood out as effective adsorbents due to their high porosity, good permeability, and sustainable character[2]. In this work, monoliths produced from a blend of cellulose acetate (CA) and cellulose acetate butyrate (CAB) were used for BPA adsorption in aqueous media. The monoliths (MCA_CAB) were produced by thermally-induced non-solvent-induced phase separation (octanol)[2] at a 3:1 CA/CAB ratio (w/w) and subsequently characterized. Adsorption was evaluated in a BPA solution (50 mg L^{-1}) by UV-Vis (λ = 276 nm) up to 400 min, using a reference monolith (MCA). Desorption tests in ethanol were performed up to 80 min in four successive cycles. As a result, in the characterization of the porous hierarchy of the monolith, N_2 adsorption analysis revealed a mesoporous structure (average pore diameter of 18.6 nm; specific surface area of 44.0 m^2 g^{-1}) embedded in a matrix with 89% macroporosity. Adsorption kinetic tests showed that the MCA_CAB monolith presented higher adsorption capacity (2.65 mg g^{-1}) than MCA (1.22 mg g^{-1}) (Figure A), possibly due to the greater hydrophobicity of CAB, since BPA presents a partition coefficient of 3.3. The process kinetics were well described by the pseudo-second-order model (R^2 = 0.998), suggesting a predominantly chemisorption mechanism. Material stability was confirmed by maintaining performance across four adsorption/desorption cycles (Figure B), demonstrating its potential for BPA removal and monolith reuse.

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(A) BPA adsorption kinetics (qt) and kinetic models. (B) Reuse of MCA_CAB in 4 cycles.

Agradecimentos/Acknowledgments

To CAPES, PROPP, FAPEMIG (process PCE-00426-25), and FINEP for financial support, and to the Multiuser Laboratory Network of the Federal University of Uberlândia (RELAM-UFU).

A QEDFT-Based Analysis of Strong Light–Matter Coupling in NTCDA

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Palavras Chave:*QEDFT,NTCDA,Light-Matter Coupling,Absorption spectrum*

Highlights

Absorption spectrum in the strong-coupling regime

Resumo/Abstract

A QEDFT-Based Analysis of Strong Light–Matter Coupling in NTCDA
NTCDA's high π-conjugation and well-defined electronic levels facilitate intramolecular charge transfer and interaction with external fields, features that are central to its for organic semiconductors, photovoltaic devices, molecular electronics, and OLEDs. Due to its highly conjugated structure and charge transfer properties, understanding NTCDA's electronic and optical properties in detail requires studying its interaction with external fields. Light-matter coupling allows for a better understanding of how these properties are modified and can be controlled at the molecular level. In optical cavities, this interaction leads to polaritons, hybrid electron-photon excitations that modify transition energies and redistribute the electronic density, offering valuable insight into the electronic dynamics under strong coupling.
In this work, we calculate the absorption spectra of NTCDA using Casida calculations and electro-photon Casida methods within linear-response Time-Dependent Density Functional Theory, as implemented in the Octopus code within the framework of Quantum Electrodynamical Density Functional Theory and employing the local density approximation (LDA) for the exchange–correlation functional. Both occupied and a broadened set of unoccupied states are considered to ensure the convergence of the electron count and oscillator strength. The analysis shows that the excitation splits into lower and upper polaritons along the photon polarization direction, while no splitting is observed in perpendicular directions, consistent with selective coupling. By varying the cavity frequency, an anticrossing between the electron–photon levels is observed, along with a redistribution of the oscillator strengths, confirming the hybrid nature of the excitations and enabling the quantification of the electron–photon composition of each polariton.

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Aumento do Teor de Biodiesel no Diesel Brasileiro: Análise do Comportamento Térmico e cinética de decomposição térmica por Termogravimetria

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Palavras Chave:*biodiesel,diesel,termogravimetria,cinetica*

Highlights

Aumento do biodiesel no diesel como estratégia nacional
Termogravimetria para avaliação de comportamento térmico
Parâmetros cinéticos de TG correlacionam com parâmetros de performance em motor

Resumo/Abstract

O aumento progressivo do teor de biodiesel no diesel constitui uma estratégia nacional para a descarbonização da matriz energética, porém impõe desafios técnicos relacionados às propriedades térmicas, cinéticas e ao desempenho de motores. Neste trabalho, avaliou-se o comportamento térmico de misturas de diesel em biodiesel comercial em diferentes proporções (BX, X = 0, 10, 20, 30, 40, 50 e 100 %v/v), por meio de análises de termogravimetria (TG/DTG) em atmosfera oxidante, com o objetivo de descrever a cinética do processo a partir do tripleto cinético: energia de ativação (Ea), fator pré-exponencial (lnA) e contribuição dos modelos cinéticos, obtidos por meio de rede neural do tipo MultiLayer Perceptron. Os resultados indicaram que o diesel puro apresenta um único evento térmico, enquanto o biodiesel puro e as misturas BX exibem dois eventos distintos, associados a etapas sucessivas de volatilização e decomposição/combustão. Observou-se que os valores de Ea e lnA aumentam de forma sistemática com a conversão e teor de biodiesel, especialmente no segundo evento. A análise dos modelos cinéticos revelou predominância de mecanismos de primeira ordem e do tipo Avrami–Erofeev de ordem 2. A partir desses parâmetros, foi possível calcular as constantes de velocidade segundo Arrhenius, sendo obtidos valores maiores para as amostras contendo biodiesel, o que indica maior eficiência do processo de combustão em motor. Os resultados indicam informações essenciais para compreender o impacto do aumento do biodiesel no diesel, estabelecendo uma base consistente para futuras correlações com parâmetros de desempenho em motores. Como perspectiva deste estudo, destacam-se os ensaios em motores utilizando as amostras B10 e B20, representativas tanto do cenário atual quanto das metas de aumento do teor de biodiesel, com o objetivo de avaliar se os parâmetros cinéticos obtidos podem ser diretamente relacionados aos parâmetros de performance em motores.

Agradecimentos/Acknowledgments

CNPq, FAPEMIG, CAPES, PPGQUI-UFMG, PPGMEC-UFMG, CTM-UFMG, CENPES/PETROBRAS

Bioengineering strategies for natural polymer-based materials: catalytic neutralization of organophosphates

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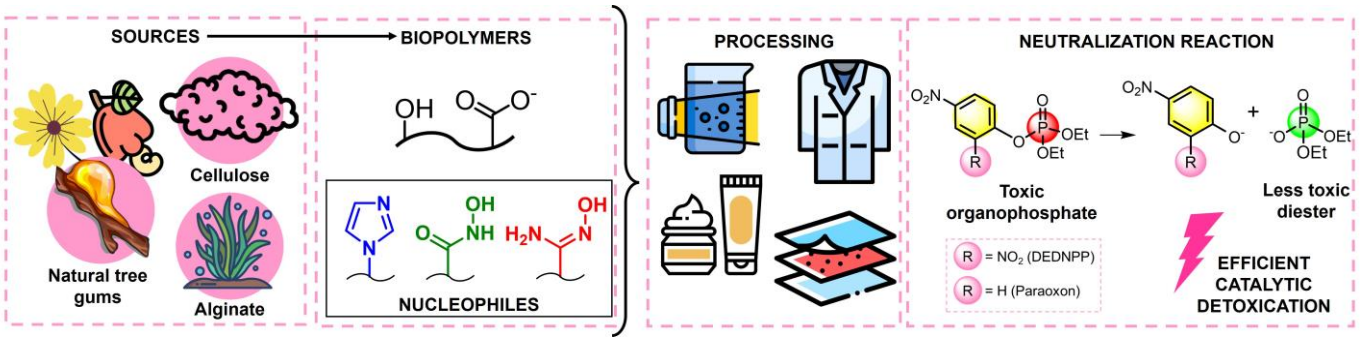
Palavras Chave:*Organophosphate, Biopolymer, Catalyst, Pesticide, Nucleophile,Organophosphate,Biopolymer,Catalyst,Pesticide,Nucleophile,Organophosphate,Biopolymer,Catalyst,Pesticide,Nucleophile*

Highlights

Efficient detoxifying materials for toxic organophosphates were achieved by the chemical anchoring of amidoxime, imidazole and hydroxamate groups onto biopolymers from different sources and forms.

Resumo/Abstract

Organophosphates pose a worldwide threat, since they are highly neurotoxic and chemically stable compounds commonly used as pesticides and chemical warfare agents. Most of the neutralization processes are time- and energy-consuming, expensive and generate byproducts – many of which are even more toxic than the precursor. Dephosphorylation reactions can promote efficient chemical detoxification through organophosphate hydrolysis but generally present drawbacks: time-consuming, low selectivity and poor recyclability – requiring a catalytic system. Exploring bioengineering through functionalization of natural polymers with (alpha)nucleophiles enables the achievement of efficient and versatile biocatalysts. Herein, we investigate the chemical modification and processing of i) commercial biopolymers (*e.g.,*carboxymethyl cellulose, alginate and hydroxypropyl methylcellulose); ii) natural tree gums (*e.g.,*buxixão gums), and iii) neutralizing gels and fabrics, with amidoximes, imidazoles and/or hydroxamates. Chemical characterization confirms the expected material features by several techniques (*e.g.,*FTIR, ^{13}C NMR, CHNS elemental analysis, TGA, potentiometric titrations, and colorimetric assays). The materials were evaluated in dephosphorylation reactions using the simulant 2,4-dinitrophenyl phosphate (DEDNPP) and the pesticide Paraoxon, revealing rate enhancements up to 10^4-fold compared with the non-catalyzed hydrolysis reaction, representing some of the best results reported in the literature. Overall, efficient and promising neutralization agents were obtained in colloidal, solid, and gel forms from commercial and waste-derived sources, promoting green, rapid, efficient, cost-effective and low-cost materials against neurotoxic organophosphates.



Schematic of the goals pursued herein

Agradecimentos/Acknowledgments

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Canard Explosion on bursts. An unexpected nonlinear dynamic behavior

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Palavras Chave:*Canard Explosion,Bursts,Oscillating reactions,Nonlinear behavior*

Highlights

Changing the flow rate value, period-2 bursts change their amplitude in a Canard Explosion behavior.

Resumo/Abstract

Several new dynamic behaviors have been observed during simulation of the chlorate-nitrous acid-iodine-iodide oscillating reaction [1] by a mechanism containing 33 chemical reactions and 27 independent chemical species. In addition to the periodic chaos [2], and burst bifurcations [3], we now report the appearance of Canard Explosion on bursts. As the k0 is increased by 1×10^{-7} s^{-1} , starting from 4.416×10^{-4} s^{-1} , the amplitude from the first and second burst (see Fig. 1a) increase or decrease, indicating the presence of the phenomena known as Canard Explosion. This is an unexpected behavior as Canard Explosion has been observed only in simple oscillations and not in bursts.

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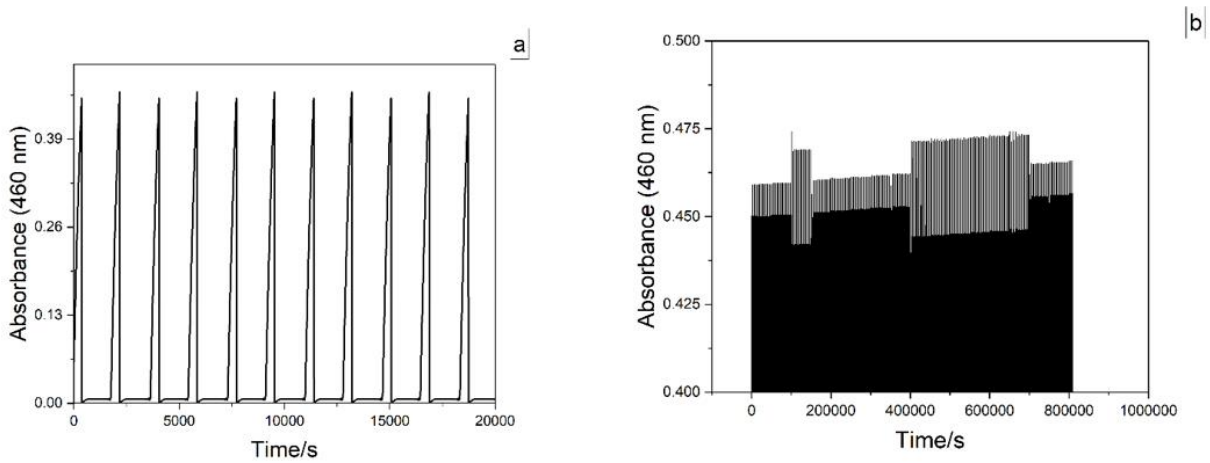


Figure 1. Canard Explosion in bursts.

Agradecimentos/Acknowledgments

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Chaotic chemical reaction models: deterministic and stochastic methods

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Palavras Chave:*chaotic chemical reactions, autocatalator, deterministic and stochastic methods,chaotic chemical reactions,autocatalator,deterministic and stochastic methods*

Highlights

We analyze the autocatalator model[1] using various methods and introduce systems derived from abstract maps that can produce simple chaotic reactions at finite scales.

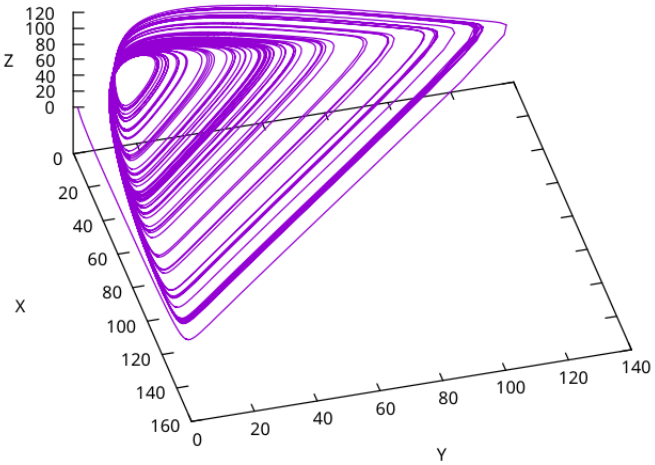
Resumo/Abstract

Chaotic chemical reactions are difficult to control, and simpler reactions could enable a more comprehensive study of these systems. We study the autocatalator model[1] using both deterministic and stochastic[2] methods and present other systems derived from abstract maps, such as the logistic map[3]. These systems can give rise to very simple chaotic chemical reactions observed under strong fluctuations. We performed several stochastic and deterministic simulations of the autocatalator model using both chemical reactions and differential equations. As the number of particles in the stochastic simulations increases, the results show smaller deviations from the deterministic approach. This shows how the number of particles affects the results. In a chaotic regime, the convergence between both methods occurs over finite time intervals. This illustrates the effects of randomness and finite-size systems on chaotic behavior. A linear stability analysis of the autocatalator shows that the model is unstable in all stationary states for the parameters considered. The analysis, however, shows stable regions. The autocatalator model with a three-molecular autocatalytic reaction is given by: P → X; P + Z → X + Z; X → Y; A + 2B → 3B; Y → Z; Z → D.

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Autocatalator (stochastic) attractor

Agradecimentos/Acknowledgments

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Chitosan microspheres containing iron oxide nanoparticles for photodynamic therapy applications

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Palavras Chave:*Magnetite, photosensitizers, singlet oxygen, release kinetics, cancer.*

Highlights

Chitosan microspheres with magnetite nanoparticles were prepared for controlled release of erythrosine, showing potential for photodynamic therapy applications.

Resumo/Abstract

Cancer is one of the leading causes of mortality worldwide.[1] Photodynamic therapy (PDT) has emerged as a promising alternative due to its selectivity and minimally invasive nature, relying on the use of light-activated photosensitizers. Erythrosine is a dye with potential application in PDT; however, its use is limited by inadequate control of its release.[2] In this context, chitosan microspheres containing magnetite may provide enhanced system stability, as well as enable controlled release and magnetic targeting. The microspheres were obtained by water/oil microemulsion polymerization. Chitosan was previously dissolved in an acetic acid solution, followed by the incorporation of erythrosine and magnetite into the aqueous phase. This phase was emulsified in an oil medium under mechanical stirring, leading to microsphere formation, which were subsequently crosslinked, neutralized, filtered, washed, and dried. Figure 1a shows the chitosan microspheres containing magnetite and erythrosine (Cs/Ery/Mag-Ms), which exhibited spherical and homogeneous morphology, with an average diameter of 77.94 µm. Figure 1b presents the erythrosine release profile at 35 °C, whose fitting using the Korsmeyer–Peppas model demonstrated excellent correlation (R^2 = 0.99), with n = 0.74 and KKP = 5.68 %·min^{-1}, characterizing an anomalous transport mechanism.[3] The results indicate that the Cs/Ery/Mag-Ms system exhibits uniform morphology and controlled release with a consistent kinetic behavior, highlighting its potential for application in photodynamic therapy.

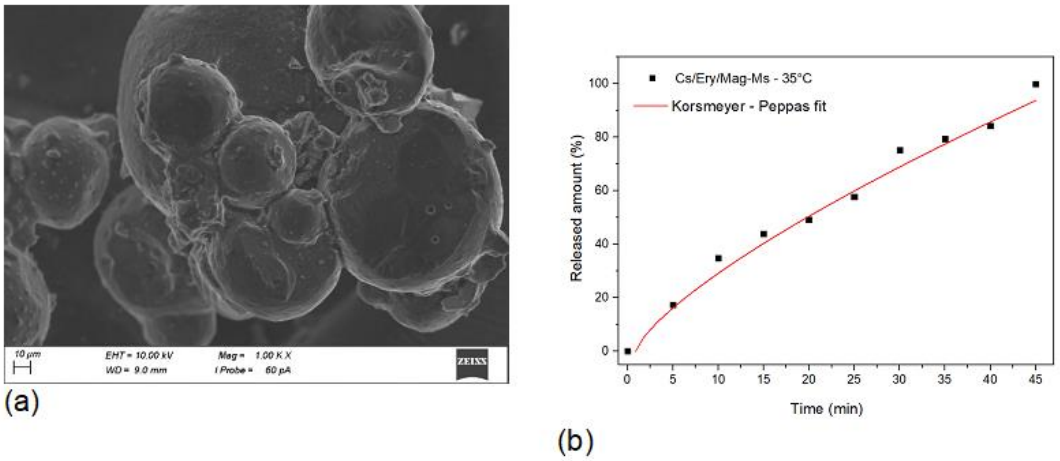


Figure 1: (a) Scanning Electron Microscopy (SEM) micrograph; (b) erythrosine release profile at 35 °

Agradecimentos/Acknowledgments

I acknowledge UNIOESTE, the GIPFEA research group, as well as the funding agencies for their financial support.

Cinética de Transferência de Carga em Sensibilizadores Orgânicos para DSSCs

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Palavras Chave:*Sensibilizadores,Energias de Reorganização,Transferência de Carga,DFT*

Highlights

Kinetic study of 10 ML-selected candidates in acetonitrile. Functional choice (wB97X-D4 vs B3LYP) critically alters charge transfer rates (kCT) and electronic coupling (V_{12}).

Resumo/Abstract

Este trabalho investiga o impacto da escolha do funcional DFT na determinação da constante cinética de transferência de carga (kCT) em Células Solares Sensibilizadas por Corante (DSSCs). O estudo partiu de uma triagem inicial de 150 moléculas em vácuo, das quais as 10 candidatas mais promissoras foram selecionadas via Machine Learning para uma análise refinada em acetonitrila. As propriedades eletrônicas, incluindo Potenciais de Ionização (IP) e Afinidades Eletrônicas (EA), foram calculadas no Gaussian 16 com a base 6-31G(d,p). O foco central, contudo, recaiu sobre a sensibilidade dos parâmetros cinéticos — energia de reorganização (λ) e acoplamento eletrônico (V_{12}), obtido via formalismo de Mulliken-Hush — frente à variação dos funcionais B3LYP, CAM-B3LYP e ωB97X-D4. Os resultados revelam que a inclusão de correções de dispersão e de longo alcance altera drasticamente a magnitude do acoplamento eletrônico e, consequentemente, do kCT. Observou-se que o funcional B3LYP tende a subestimar a velocidade de transferência de carga para a maioria dos sistemas (notavelmente na molécula D4B5A2), enquanto o ωB97X-D4 oferece uma descrição distinta, invertendo o comportamento em casos específicos como o D2B1A1. Conclui-se que a precisão na predição da injeção de carga é severamente dependente da metodologia teórica empregada: a escolha inadequada do funcional pode levar a desvios de ordens de grandeza no kCT, comprometendo a validação de candidatos a fotossensibilizadores.

Agradecimentos/Acknowledgments

CAPES, CNPq, UnB, FAP-DF, LMSC, LQC, LEEDMOL

Classification of crude and weathered Brazilian oils: an analysis based on SFT dispersibility results

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Palavras Chave:*Oil spill, Weathering process, Chemical dispersant, Swirling Flask Test,Oil Spill,Weathering Process,Chemical Dispersants,Swirling Flask Test*

Highlights

Chemical dispersants mitigate oil spills at sea.
The weathering process affects dispersion effectiveness.
SFT is the standard methodology used to determine chemical dispersant effectiveness in Brazil.

Resumo/Abstract

Offshore petroleum exploration growth has heightened concerns regarding oil spills and their resulting impacts on marine ecosystems and local economies (Zacharias, 2020). When released in the sea, oil undergoes weathering — a combination of physical, chemical, and biological processes that alter its composition (Adofo et al., 2022). While chemical dispersants are vital mitigation tools, their effectiveness is hindered by weathering, which increases viscosity and promotes emulsion formation (Dalinge*t al.*, 1990).

Understanding the evolution of the physical-chemical properties of spilled oil is essential to determining the appropriate timing for dispersant application (Venosa, 2013; Singh*et al.*, 2020). This study aims to evaluate similarities among crude and weathered Brazilian oils and to propose a classification system based on dispersibility. Three groups were identified in the sample conjunct throughout a Principal Component Analysis (PCA). The first principal component (PC1) differentiates samples mainly according to their density (°API), whereas the second principal component (PC2) is correlated with the weathering influence.

These groups were categorized as dispersible, partially dispersible, or non-dispersible, following effectiveness criteria established by Normative Instruction 7 (IBAMA, 2001) via the SFT (Swirling Flask Test). These results summarize the dispersibility tendencies among the analyzed samples and suggest a preliminary step for categorizing oil behavior within the Brazilian context.

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Agradecimentos/Acknowledgments

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Coaxial electrospinning of polysaccharides: polymer and parameter evaluation.

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Palavras Chave:*1- Melhorar as palavras-chave como exemplo: 'Coaxial electrospinning; nanofibers development' 2- Em "For PCL (core) and PVA/Starch in both positions, results were satisfactory due to the difference in solvent volatility. " Esta conclusão foi muito evasiva, sem evidência experimental. Os resultados foram satisfatórios por quê? Eles favoreceram a rápida solidificação? As fibras se formaram sem grânulos? Houve separação de fases? Ou formação de uma estrutura núcleo–casca bem definida? Por favor, corrija,nanofibers development,Coaxial electrospinning,Chitosan,Starch*

Highlights

Coaxial polysaccharides nanofibers
Stable coaxial fibers were produced using a PCL core and PVA-starch shell
Future morphological and chemical tests will determine potential applications

Resumo/Abstract

Polysaccharides are sustainable, biodegradable, low-toxicity macromolecules consisting of monosaccharides connected by O-glycosidic bonds. They are promising for electrospinning, a versatile technique for producing nanofibers. However, uniaxial electrospinning of pure polysaccharides is challenging due to their viscoelasticity and molecular structure. This work aims to develop nanomaterials via coaxial electrospinning, optimizing parameters to obtain stable nanofibers from different polysaccharides.The PVA/starch solution was obtained by dissolving PVA at 90°C and gelatinizing starch at 65°C, with subsequent addition of sorbitol. The chitosan/PVA solution was prepared from chitosan in acetic acid and PVA with citric acid, combined in a 70/30 ratio. Ethylcellulose was dissolved in a DMA/THF mixture. Polycaprolactone (PCL) was dissolved in a DMF and chloroform mixture. All preparations were carried out under stirring to ensure complete solubilization. For the electrospinning of PVA/starch and chitosan/PVA in both positions (core or shell), the formation of fibers with phase separation was not observed, explained by the low volatility of the common solvent (water), which prevents rapid solidification. For PVA/Starch and ethylcellulose, fiber formation occurred without the presence of beads, but electrospinability decreased over time, indicating possible solution instability. For PCL (core) and PVA/Starch in both positions, results were satisfactory: uniform fibers without beads were observed by optical microscopy, favored by the difference in solvent volatility. Additionally, confirmation of a well-defined core–shell structure with phase separation between the components is still under investigation using techniques such as TEM and FTIR.

Agradecimentos/Acknowledgments

The authors would like to thank the GIP&FEA–Unioeste, CAPES, CNPq, INCT Polysaccharides. ARSR thanks the CNPq for the Postdoctoral fellow provided by the INCT Polysaccharides program.

Colorimetric Detection of Pesticides Based on Derivatization at Nitrogen Sites

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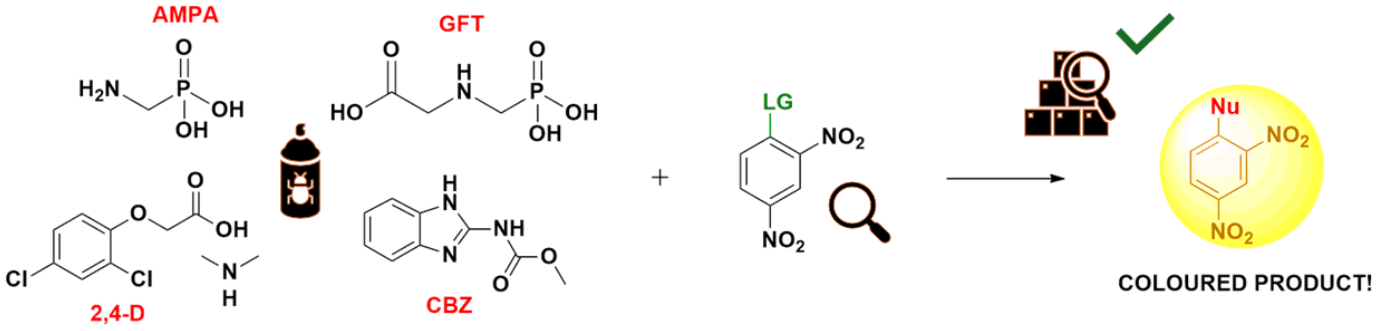
Palavras Chave:*agrochemicals,organophosphates,glyphosate,pesticides monitoring*

Highlights

Kinetic and spectroscopic investigation of nitrogen-based derivatization reactions applied to pesticide detection; Development of a simple and low-cost colorimetric method for pesticides' monitoring.

Resumo/Abstract

Pesticides play an important role in agricultural production. However, their extensive use may pose risks to the environment and human health, especially in the case of organophosphate compounds. In addition, the detection of these substances is often challenging due to the complexity of analytical matrices and the cost and sophistication of conventional methods. Therefore, this study aims to develop a simple, selective, and cost-effective colorimetric method for the detection of pesticides, including the organophosphates glyphosate (GFT) and its main metabolite aminomethylphosphonic acid (AMPA), as well as carbendazim (CBZ) and the amine salt of 2,4-dichlorophenoxyacetic acid (2,4-D). The proposed approach relies on derivatization reactions occurring at nitrogen-containing functional groups of the analytes, using activated 2,4-dinitrophenolic compounds to form colored products. The reactions were monitored by UV-Vis spectroscopy, and product formation was confirmed by the appearance of absorption bands in the 300-400 nm spectral region, supported by kinetic studies. For GFT and AMPA, the method showed high selectivity in alkaline conditions, enabling the clear differentiation between both compounds, even when simultaneously present in the same sample. These results supported the development of a colorimetric sensor capable of selectively detecting these organophosphates. The same derivatization strategy is being extended to carbendazim and 2,4-D amine salt, with ongoing studies focused on reaction kinetics, selectivity, and analytical performance. Complementary NMR analyses are being conducted to support the understanding of the derivatization mechanism. Overall, the developed colorimetric approach provides a promising tool for pesticide monitoring, especially for rapid and low-cost analyses in complex samples, without the need for sophisticated instrumentation or extensive sample pretreatment.



Generic representation of the proposed mechanism for derivatization.

Agradecimentos/Acknowledgments

UFPR, CAPES, CNPq, Fundação Araucária, NAPI SP/CF, PhosAgro/Unesco/IUPAC, L'Oréal-UNESCO-ABC, INCT NanoVida, INCT Nanocarbono e Materiais 2D.

Combining Molecular Dynamics and Electronic Structure Methods to Describe Spin Relaxation in an Ionic Liquid

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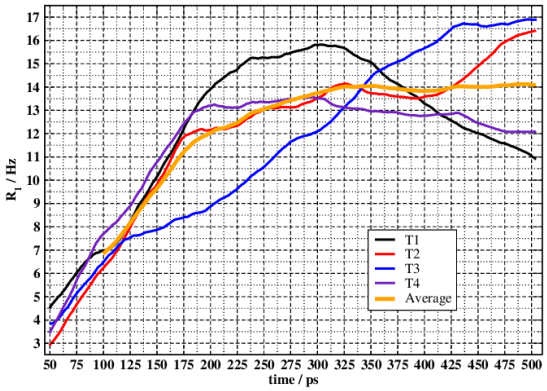
Palavras Chave:*ab initio molecular dynamics,DFT,quadrupolar relaxation,ionic liquid,ethylammonium nitrate.*

Highlights

This is the first study focosed on the quadrupolar relaxation in an ionic liquid described by one solvation shell shows an error of 4%, while with only implicit solvation the error increases to 30%.

Resumo/Abstract

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful and widely used technique for obtaining structural information from organic and inorganic compounds, whether through chemical shifts, indirect spin-spin coupling constants, or quadrupole interactions. In NMR experiments, the kinetic behavior of the system's magnetization is commonly described by Bloch's equations, which have as basic parameters the longitudinal (T1) and transverse relaxation times, or their respective rates, R1 = 1/T1 and R2 = 1/T2. This work presents a methodology for the ab initio calculation of relaxation times for nuclei with electric quadrupole moments (I>1/2) in ionic liquids. In quadrupolar nuclei, the relaxation properties are determined by the autocorrelation function of the electric field gradient (EFG) acting on the nucleus, more precisely by its spectral density, together with the magnitude of the nuclear quadrupole moment and the spin quantum number. To describe the temporal evolution of electron density on the quadrupolar nucleus due to vibrational motion and interactions with neighboring molecules, we used ab initio molecular dynamics, with the electronic structure described by PBE functional. The system chosen was ethylammonium nitrate, triply deuterated at the cation's amino group (NEA-D3). Clusters containing the cation and two solvation spheres were extracted at regular time intervals, and the EFGs of the deuteriums were calculated using wB97X-V functional, which also includes dispersive interactions, and the ma-def2-TZVP basis set. Implicit solvation given by the SMD model was used in these clusters. Relaxation in NEA-D3 occurs in the so-called Extreme Narrowing Regime, meaning that T1=T2. The value obtained for 1/T1 was 13.3 ± 1.0 Hz, approximately 60% higher than the measured value. It is worth noting that the present study has accuracy similar to, or even better than, that of previously conducted studies on systems not involving ionic liquids.



Isotropic longitudinal relaxation rates computed for the four independent trajectories.

Agradecimentos/Acknowledgments

We acknowledge LNCC/MCTI, Brazil, SDumont supercomputer, CENAPAD--SP, CCR-UB for providing computational HPC resources. FAPESP, CNPq, CAPES and NSC.

Comparative Thermodynamic Analysis of TT, B, and T Phases of Nb_2O_5

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Palavras Chave:*Niobia, DFT+U, Phonons, Phase Transition,Niobia,DFT+U,Phonons,Phase Transition*

Highlights

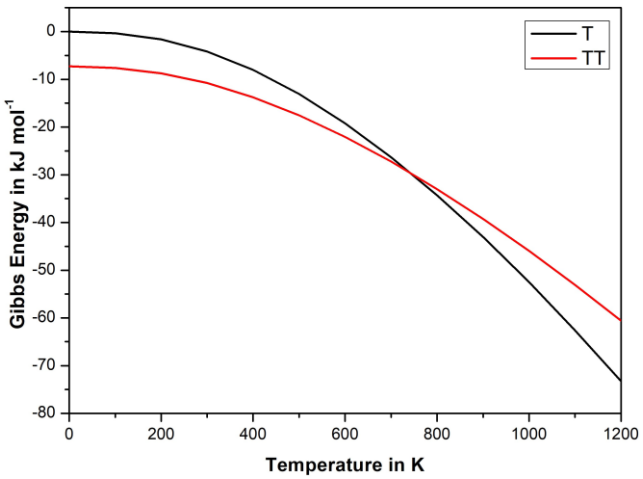
Detailed DFT characterization of pseudo-hexagonal TT-Nb_2O_5.

Thermodynamic comparison of TT, B and T phases via phonon calculations.

The TT→T transition temperature agrees with experiment.

Resumo/Abstract

Niobium is a strategic element with wide technological applications, particularly in energy storage and catalysis. Brazil holds approximately 98% of the world's reserves, underscoring the importance of understanding the structure of its source minerals. Niobium oxide exhibits polymorphism at room temperature, forming different crystalline phases depending on thermal conditions. The TT phase is the first to form at low temperatures and remains poorly characterized, while higher temperatures promote transformation into more thermodynamically stable phases. This work focuses on the detailed structural and electronic characterization of pseudo-hexagonal TT-Nb_2O_5 in its crystalline form, as well as a comparative thermodynamic analysis of the B, T, and TT phases to identify the stability and phase transition temperatures and correlate them with experimental data. Density Functional Theory (DFT) calculations were performed using the Quantum Espresso package with the PBE exchange–correlation functional. A plane-wave cutoff energy of 60 Ry and a 4×2×4 Monkhorst–Pack k-point mesh was employed for all systems. For TT-Nb_2O_5, different vacancy configurations were explored to obtain the stoichiometric Nb_2O_5 composition. The Hubbard parameter varied from 0 to 9 eV, and 9 eV was selected as provided the best agreement with the experimental band gap. Thermodynamic properties were evaluated through phonon calculations, enabling a comparison of the relative stability of the TT, B, and T phases. The TT-T phase transition temperature was determined to be 740 K, in agreement with available experimental data (683-873 K). The B-T transition was also examined. Since the TT phase is the first to form at lower temperatures, its detailed characterization is essential for understanding the structural and electronic behavior of Nb_2O_5 and for establishing a reference framework for comparison with other phases.



Gibbs Energy vs. Temperature for the TT and T phases of Nb_2O_5

Agradecimentos/Acknowledgments

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Computational Analysis of CDK2 and ULK1/2 Inhibitory Compounds

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Palavras Chave:*Selective Inhibitors; Computational Modeling; DFT; Autophagy*

Highlights

DFT calculations show that the kinase inhibitors exhibit high affinity for the active sites of the kinases.

Resumo/Abstract

This work presents a computational approach to investigate BLU-222 and DCC-3116 as novel kinase inhibitors. BLU-222 is a potent and selective inhibitor of the cyclin-dependent kinase CDK2, whereas DCC-3116 is an experimental modulator of the serine/threonine kinases ULK1 and ULK2, key regulators of autophagy. The aim of this study is to examine the structural and electronic properties, solvation stability in water and DMSO, spectroscopic behavior, and interaction potential with biological targets. The methodology relies on density functional theory (DFT) calculations to optimize the ground-state geometry, obtain harmonic frequencies, and determine conformer energies to identify the most stable structure. The B3LYP, M06, and ωB97X-D functionals were employed with the 6-311+G (2d, p) basis set in the gas phase and in implicit solvents. Time-dependent DFT (TD-DFT) was used to predict UV-Vis spectra and the HOMO-LUMO gap, highlighting the main electronic transitions and their relationship with molecular structure. The results indicate that B3LYP yields the lowest energies and is therefore the most suitable functional for describing both BLU 222 and DCC 3116. Solvation strongly stabilizes both molecules (with B3LYP being most stabilizing for BLU 222 and ωB97X D for DCC 3116), and the TD DFT UV vis spectra display several intense bands in the UV region that provide a useful qualitative model in the absence of experimental data. Table 1 summarizes the solvation energies in water and DMSO, while Figure 1 shows the optimized geometries, confirming the minimum energy conformations used for the electronic property calculations.

Compound	Functional	ΔEsolv Water (kcal·mol⁻¹)	ΔEsolv DMSO (kcal·mol⁻¹)
BLU-222	B3LYP	−17,907	−19,638
BLU-222	M06	−15,507	−17,432
BLU-222	ωB97X D	−16,719	−19,300
DCC-3116	B3LYP	−20,478	−22,561
DCC-3116	M06	−17,892	−20,164
DCC-3116	ωB97X D	−20,763	−23,424

Table 1: DFT Solvatation energies(ΔE, kcal·mol⁻¹)of BLU-222 and DCC-3116 in water and DMSO(Smd model)

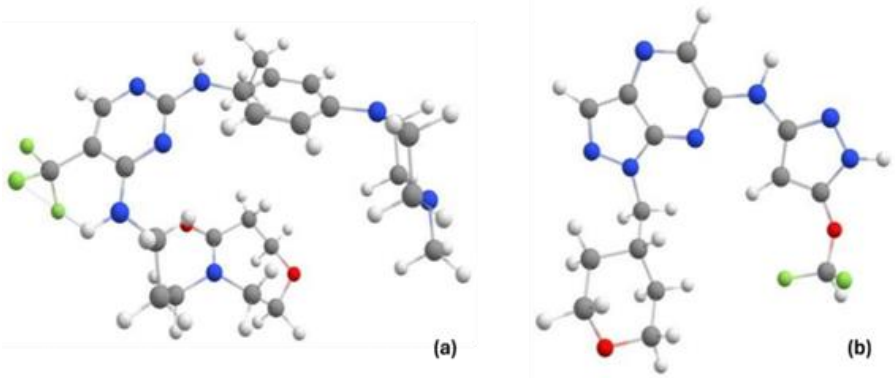


Figure 1. Optimized structures of the compounds DCC-3116 (a) and BLU-222 (b).

Agradecimentos/Acknowledgments

1. Conselho Nacional de Desenvolvimento Científico e Tecnológico; 2. Fundação de Amparo à Pesquisa do Estado de Minas Gerais; 3. Programa de Pós-Graduação em Química da Universidade Federal de Juiz de Fora; 4. Núcleo de Estudos em Química Computacion

Computational study of the electronic structure of a manganese (I) complex.

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Palavras Chave:*Fotossensibilizador de Manganês (I), HOMO-LUMO, DFT.,Fotossensibilizador de Manganês (I), HOMO-LUMO,Fotossensibilizador de Manganês (I), HOMO-LUMO, DFT*

Highlights

Exploring the electronic structure of Mn(I) complexes via DFT methods.

Resumo/Abstract

The search for photosensitizers based on abundant 3d-series metals has focused on developing Manganese(I) complexes to replace noble metals. Recently, the $[Mn(pbmi)_2]^+$ complex (Figure 1a) showed outstanding photophysical properties. This work presents a density functional theory (DFT) study of this complex. X-ray data were used to select the best functional from those tested: BP86-D3(BJ), PBE-D3(BJ), M06-L, B3LYP-D3(BJ), B3PW91-D3(BJ), B3P86-D3(BJ), M06, PBE0-D3(BJ), CAM-B3LYP-D3(BJ), and ωB97X-D3(BJ). All calculations used the def2-TZVP basis set. "D3(BJ)" shows where dispersion correction was incorporated. M06 and PBE0-D3(BJ) functionals showed the smallest structural deviations. After functional selection, solvent effects were modeled using CPCM (acetonitrile). Regardless of solvent, the HOMO orbital has a metallic character, and the LUMO is delocalized over the polypyridine ligands. This suggests that the lowest-energy transition is MLCT (metal-to-ligand charge transfer; Figure 1b).

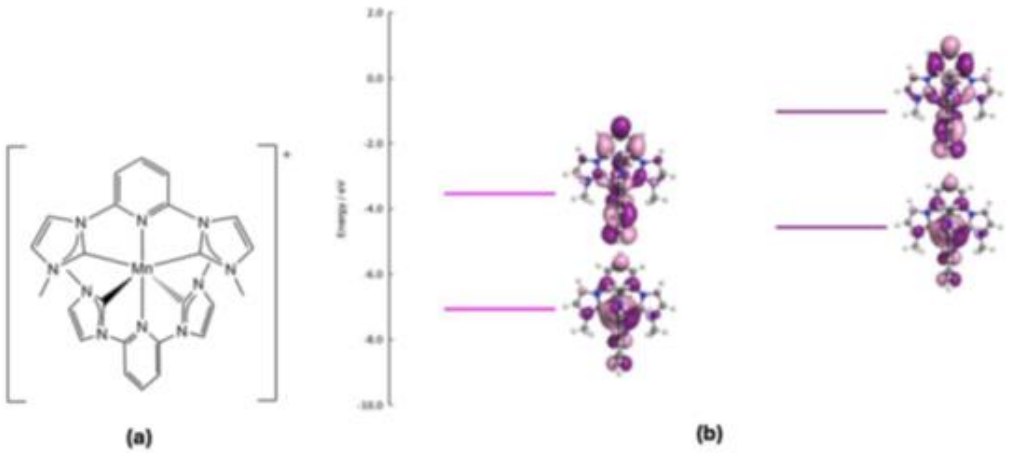


Fig 1: (a) [Mn(pbmi)2]+; (b) HOMO-LUMO (GS) M06/def2-TZVP in gas (left) and acetonitrile (right).

Agradecimentos/Acknowledgments

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Computational Study of Tryptophan/β-Cyclodextrin Complexation

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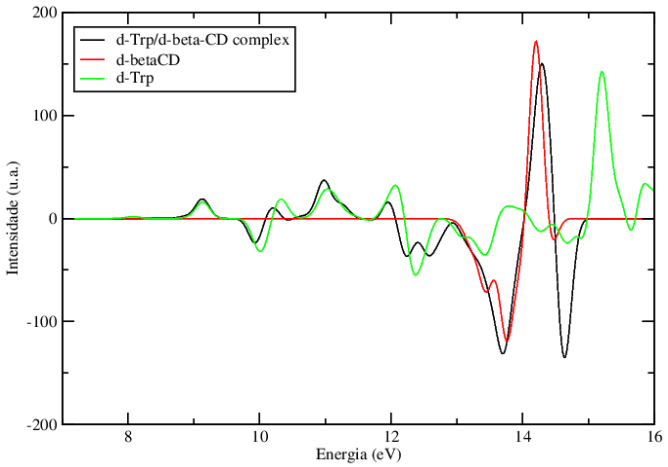
Palavras Chave:*β-Cyclodextrin, Circular Dichroism, Inclusion Complexes, Tryptophan*

Highlights

This computational Circular Dichroism study reveals how Tryptophan's chirality influences thestability and enantioselective interactions in its β-cyclodextrin inclusion complexes.

Resumo/Abstract

β-Cyclodextrin (*d*-β-CD) is a cyclic oligosaccharide capable of forming inclusion complexes that can modify the solubility, stability, and physicochemical properties of guest molecules, and it is widely used in the pharmaceutical, cosmetic, and food industries [1]. Spectroscopic data that describe how the chirality of the guest molecule affects the stability of these complexes are essential for a detailed understanding and for improving their applications. Recently, the synthesis of*l*-β-cyclodextrin [2] has opened new possibilities, complementing those of its widely used enantiomer. In this work, we present a computational Circular Dichroism study of the isolated molecules and of the tryptophan/β-cyclodextrin complex, aiming to investigate the underlying interactions, enantioselectivity, and stability. Geometries were optimized in vacuum using the GFN2-xTB program [3], and the spectra were obtained with ORCA using the semiempirical ZINDO-CI method, with single excitations and 250 roots. In the figure, we show an example of the results for the d-β-cyclodextrin/d-tryptophan complex in comparison with the spectra of the isolated molecules. The bands observed for the isolated species are also present in the complex spectrum, albeit with intensity changes and energy shifts that reflect the nature of the interactions. Results covering all enantiomeric combinations will be presented during the event.



Circular Dichroism spectrum of pure d-Tryptophan and d-βCD, and of the Tryptophan/β-CD complex

Agradecimentos/Acknowledgments

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Conjugation Effects in Mn(I) PhotoCORMs

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Palavras Chave:*PhotoCORMs,Mn(I) complexes,Metal-CO bonding,EDA-NOCV,DFT*

Highlights

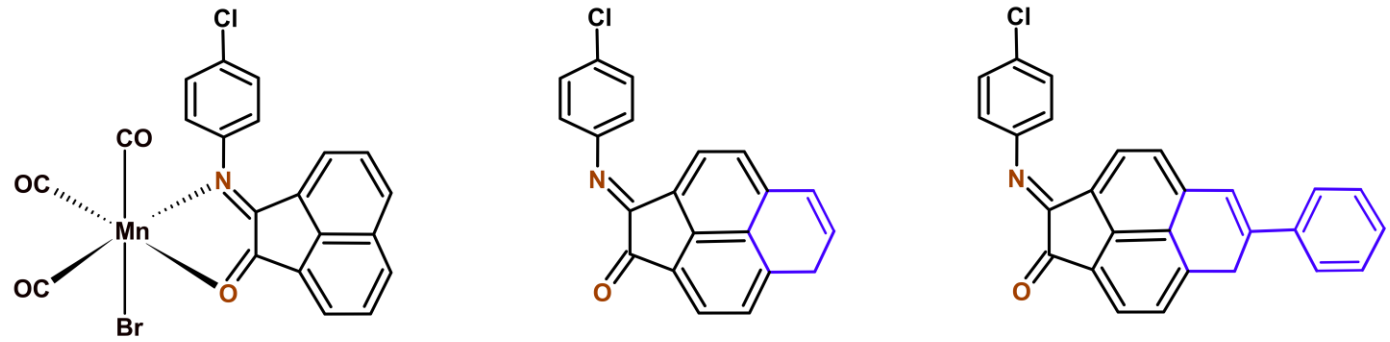
Ligand π-conjugation effects on Mn(I) photoCORMs. EDA-NOCV analysis of Mn-CO interactions. Electronic structure modulation related to CO release.

Resumo/Abstract

Photoactivated carbon monoxide releasing molecules (photoCORMs) based on Mn(I) tricarbonyl complexes have attracted growing interest due to their potential for controlled CO delivery and tunable photochemical behavior. In this work, the effects of ligand π-conjugation on the ground-state electronic structure of Mn(I) photoCORMs are investigated using the complex [$MnBr(CO)_3$(MIAN)] as a reference system, where MIAN = 2-[(4-chlorophenyl)imino]acenaphthylen-1-one, a conjugated α-diimine ligand. Structural modifications of the ligand framework are proposed to systematically assess how conjugation influences metal-ligand interactions and Mn-CO bonding.

The ground-state electronic structure will be studied using density functional theory (DFT). The nature of Mn-CO bonding will be analyzed through Energy Decomposition Analysis combined with Natural Orbitals for Chemical Valence (EDA-NOCV), allowing a quantitative description of the σ-donation and π-backdonation contributions and their dependence on ligand conjugation. This approach enables the assessment of how electronic delocalization within the ligand framework affects metal-CO backbonding and, consequently, the sthength of Mn-CO interaction. This study aims to elucidate the role of ligand π-conjugation in modulating the electronic structure and Mn-CO bonding in Mn(I) photoCORMs. the combined DFT and EDA-NOCV analysis is expected to provide molecular-level insight into structure-property relationships, contributing to the rational design of Mn(I) photoCORMs with improved and tunable CO-release properties.

(a) (b) (c)



(a) [$MnBr(CO)_3$(MIAN)]. (b–c) π-extended MIAN ligands for Mn(I) PhotoCORMs.

Agradecimentos/Acknowledgments

FAPESP (2022/12043-5 and 2025/16402-8) and CAPES(001).

Controlling produced water quality in the petroleum industry: effects of chemical additives, pH and temperature.

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Palavras Chave:*Compatibility,Colloids,Iron oxide,Precipitate,Coagulant*

Highlights

Increasing temperature and pH accelerates precipitation.

Corrosion inhibitor reduces precipitate size, while coagulant increases it.

The other tested additives do not affect the precipitate.

Resumo/Abstract

Produced water management is complex due to its variable composition and growing environmental concerns. This study examines its colloidal structure and the impact of chemical additives, focusing on the synergistic or incompatible interactions that dictate treatment efficiency and facility integrity.

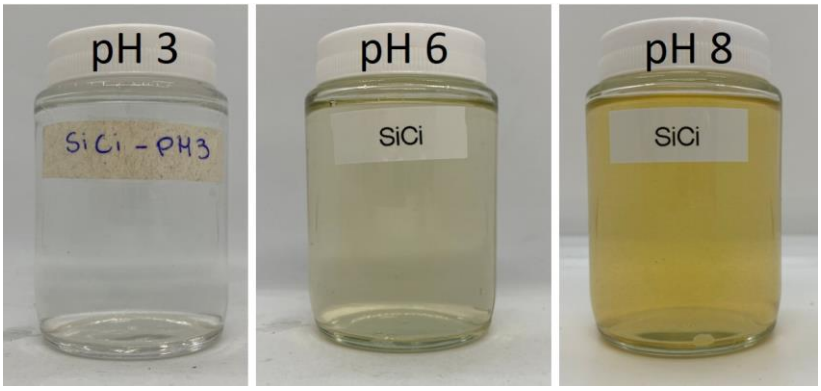
In this study, the effects of different types of additives were evaluated in a synthetic brine: scale and corrosion inhibitor, defoamer, demulsifier, coagulant, and flocculant. The effects were observed over 12 hours at pH 3, 6, and 8 and at temperatures of 24 and 60 °C. The concentrations and components used to prepare the synthetic brine were based on the composition of real samples of produced water, which presented turbidity problems on the platform.

An orange solid immediately precipitated when all the samples were adjusted to pH 8. The same precipitate was observed in the brines after 12 hours at 60 °C, at pH 6. In samples at pH 3, the precipitate did not form at room temperature, even after 12 h; it formed only at 60 °C in the presence of the coagulant. The solid was identified as iron oxide/hydroxide.

When comparing pure brine with brine containing a corrosion and scale inhibitor at pH 8, the precipitate particle size in the inhibitor-containing sample is visibly smaller. The same phenomenon does not occur at pH 6. The only change in particle size occurs in the presence of the coagulant.

The results indicated that increases in temperature and pH induce the formation of a precipitate responsible for the turbidity of the produced water. The precipitate is mainly composed of iron oxides/hydroxides. The corrosion and scale inhibitor increases its dispersibility, while the coagulant promotes larger particles. The other additives do not affect the precipitate.

In conclusion, the study identifies parameters to control solid formation in oil industry produced water, which is crucial for optimizing additive use and preventing operational problems.



Particle size increase with increasing pH.

Agradecimentos/Acknowledgments

The authors thank Shell Brasil for financial support through the R, D&I ANP clause (ANP project number 23016-9)

coor2graph: A Tool for Graph-Theoretical Analysis of Molecular Simulation Data

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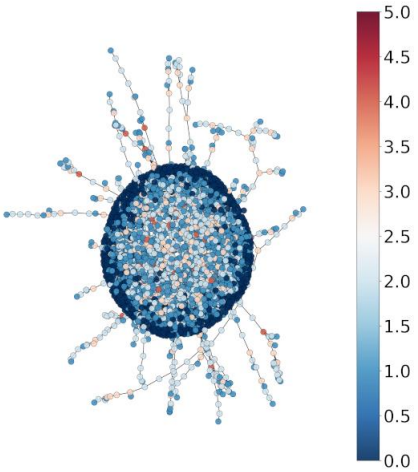
Palavras Chave:*graphs,Interface Fortran-Python,Molecular Dynamics,Monte Carlo Simulation*

Highlights

Graphs-based molecular simulation analysis

Resumo/Abstract

Graph theory and the study of complex networks provide a conceptual framework for describing molecular structures, reactivity, and interactions in a unified manner, enabling the identification of structural and dynamic patterns relevant to understanding complex chemical systems. Within this approach, molecular systems can be described as graphs, where atoms, molecules, or interaction sites correspond to nodes and molecular interactions are represented as edges defined according to topological or geometric criteria, energetic thresholds, or dynamical correlations. In this representation, both static and dynamic properties of the molecular system, such as coordination numbers, connectivity, and collective interactions, can be analyzed using graph-theoretical measures. We present coor2graph, a Fortran-based program with a Python interface for the analysis of complex networks derived from molecular dynamics and stochastic simulation trajectories. The program analyzes molecular positions to obtain user-defined adjacency matrices, which are then passed to the Python library NetworkX, where graph measures are calculated. Coor2graph is an open-source, free, parallelized Fortran-Python program that can be compiled using the GNU Fortran Compiler on different GNU/Linux distributions, is licensed under the GPLv3 license, and is available at github.com/aslozada/coor2graph.
In the current version of coor2graph, calculations of adjacency matrices between pairs of sites, special cases with three sites, and two- or three-dimensional lattices are available. The program also provides options for analysis under various periodic boundary conditions, and the interface with the Python NetworkX library allows the calculation of graph measures such as degree, closeness, betweenness, eigenvalues, and harmonic centrality. In addition, coor2graph interfaces with Python plotting libraries to generate graphical representations of the graphs for visualization and further analysis.



Graphs displaying the water TIP3P complex network and color-based on the respected degree_centrality

Agradecimentos/Acknowledgments

This research was supported by HPC resources provided by the Superintendência de Tecnologia da Informação of the University of São Paulo.
FAPESP (grants 2023/09350-6)

Development of a combined experimental and theoretical methodology for stereochemical determination of piperidine alkaloids from Senna spectabilis

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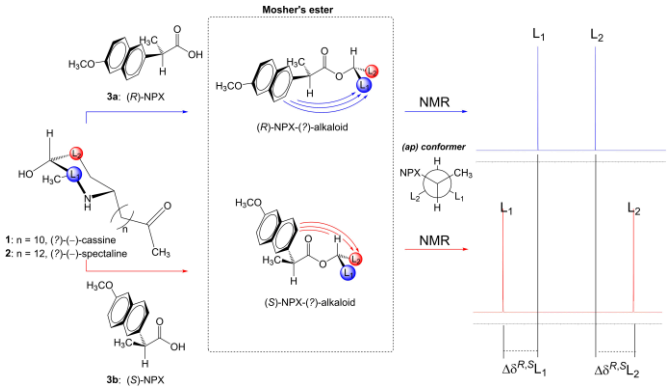
Palavras Chave:*Senna spectabilis,stereochemistry,computational chemistry,conformation,Mosher's esteres*

Highlights

Experimental and theoretical ^{13}C NMR established stereochemistry of*Senna spectabilis*alkaloids.
DFT ^{13}C NMR supported experimental analysis.
DMBO low-energy conformers aided Mosher's ester analysis.

Resumo/Abstract

Senna spectabilis is a source of chiral piperidine alkaloids that have proven to be active as antimalarials, anti-chikungunya and anticholinesterase, a key enzyme in Alzheimer's disease. This pharmacological potential is associated with the chiral piperidine alkaloids (−)-cassina (**1**) and (−)-spectaline (**2**). Elucidating the absolute stereochemistry of these compounds using literature methods (IR and XRD) can present practical limitations. Therefore, this work aims to develop a methodology for the stereochemistry assessment of**1**and**2**, using NMR analysis and a chiral derivatizing agent (CDA), which in this study was (S)-naproxen (**3**), an efficient and lower-cost alternative to the classic Mosher reagent. Computational studies were also performed to contribute to the determination of the main conformers and to assist in establishing the positions of the substituents on the piperidine nucleus. Furthermore, the anisotropic effects (shielding/deshielding) of the naphthyl ring of**3**on the neighboring groups of the stereogenic center are essential to establish the absolute configurations (AC) of**1**and**2**. After isolating the alkaloids, Steglich esterification was performed using**3**and its racemic form, the latter obtained by acid-catalyzed racemization to generate esters for comparison with the computational conformational analysis. The study of the conformational space was performed using the GNF2-xTB quantum dynamics method. The simulation was conducted with a duration of 1 ns in the NVT ensemble. The solution environment was reproduced using the ALPB implicit solvation model parameterized for the chloroform solvent. The calculations indicated that the most stable (ap conformer) exhibits a ΔG of 40 kJ.mol^{-1} relative to the sp conformer, providing the structural basis for interpreting the NMR spectra. These results demonstrate the feasibility of using**3**combined with computational conformational analysis as an accessible strategy for stereochemical assignment of**1**and**2**.



Double derivatization method using 3 as CDA for assignment of the absolute configuration of 1 and 2.

Agradecimentos/Acknowledgments

Acknowledges CNPq, CAPES, INCT-BioNat and FAPEMIG for fellowships.

Development of Biomimetic Lipid Nanoparticles: Physicochemical Properties and Cellular Uptake Dynamics

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Palavras Chave:*Drug delivery Lipossomas híbridos, Estabilidade coloidal, DLS, Potencial Zeta,Drug delivery,Lipossomas híbridos,Estabilidade coloidal,Potencial Zeta,Espalhamento Dinâmico da Luz*

Highlights

Conventional and biomimetic liposomes differ in physicochemical properties and uptake cellular dynamics. Liposomes coated with tumor or erythrocyte membranes enable distinct therapeutic applications.

Resumo/Abstract

A incorporação de membranas celulares em nanossistemas é uma estratégia promissora para conferir propriedades biomiméticas a nanopartículas, otimizando sua estabilidade e biodistribuição. Este estudo desenvolveu lipossomas híbridos (hLPs) funcionalizados com membranas de eritrócitos (RBCs) ou de células tumorais B16.F10 (mB16), visando modular a evasão imunológica e o direcionamento celular.

As formulações foram preparadas por hidratação de filmes lipídicos (70% fosfatidilcolina, 30% colesterol) a 5 mM, seguida de extrusão. Foram obtidas três amostras: controle (PC), híbrido com eritrócitos (RBC-PC) e híbrido com mB16 (B16-PC), na proporção 5:1 (lipídeo:membrana). A hibridização ocorreu via ciclos de congelamento–descongelamento. A caracterização por DLS indicou diâmetro próximo a 150 nm (± 10 nm) e PDI < 0,2, demonstrando estabilidade coloidal e homogeneidade. A hibridização alterou o potencial zeta de –27 mV (PC), para –30 mV (RBC-PC) e –44 mV (B16-PC), indicando a hibridização das hLPs.

A internalização celular foi avaliada por citometria de fluxo em linhagens B16.F10 (tumoral) e J774A.1 (fagocítica). Em B16.F10, a B16-PC mostrou captação superior em 0,5, 1 e 4 h (2,8%, 5,6% e 13,3%), seguida por RBC-PC (1,6%, 2,1% e 2,4%) e PC (0,4%, 0,4% e 0,5%). Em J774A.1, a captação foi distinta para B16-PC (27,2%, 39,8% e 89,1%) e RBC-PC (13,9%, 25,2% e 100%), contra o controle PC (3,2%, 3,8% e 8,5%).

Os resultados indicam que a hibridização altera o perfil das interações biofísicas e o perfil de internalização. A membrana tumoral potencializa o reconhecimento homotípico, enquanto a de eritrócitos confere maior furtividade inicial e perfil de internalização

Effect of UV-C photodegradation on Poly (lactic acid) (PLA)

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Palavras Chave:*Poly(lactic acid),UV-C,Photodegradation,Rheology,FTIR*

Highlights

FTIR ester index tracks UV-C-induced O–C bond cleavage in PLA at different temperatures; increasing irradiation time lowers rheological viscosity.

Resumo/Abstract

Fossil fuel–based plastic waste materials have become major contributors to environmental pollution in recent years. To minimize the impact of these materials, bio-based and biodegradable polymers have emerged as a feasible alternative. Among them, poly(lactic acid) (PLA) exhibits outstanding properties, with stiffness, strength, and gas permeability comparable to those of conventional petrochemical-based polymers. As a result, disposable fossil fuel–based plastic products, such as food packaging, biomedical devices, textiles, and electronics, have been progressively replaced by PLA due to its properties and biodegradability. Despite its outstanding properties, PLA is sensitive to UV radiation and undergoes photodegradation when exposed to this wavelength, impacting its properties and its devices life-span. Therefore, in this study, the effects of UV-C radiation and temperature on PLA photodegradation were investigated. Rheological measurements showed that UV irradiation affects PLA viscosity, which decreases with increasing exposure time. Infrared spectroscopy revealed changes in the ester bonds, indicating chain scission upon UV exposure. Exposure temperature also influenced both rheological viscosity and FTIR results. Overall, the results indicated that PLA is sensitive to UV radiation and temperature, which significantly affect its degradation behavior.

Agradecimentos/Acknowledgments

FAPESP (2025/06511-4), (CAPES (0001), INCT-Circularidade and CNPq (384749/2025-9), UFSCar, PPGQ, DQ.

Effects adsorption and doping of metallic atoms on d-MoC(001) surface

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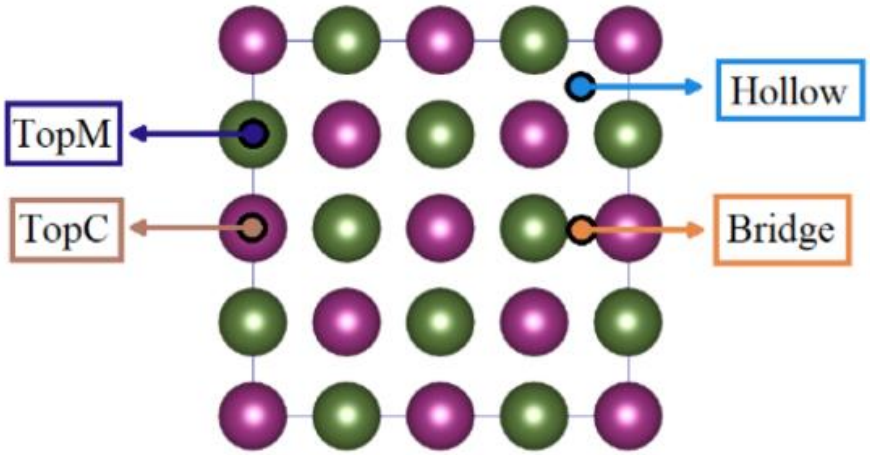
Palavras Chave:*Adsorption, transition metal carbides, electronic structure, density of states, doping effect,Adsorption,Transition Metal Carbides,Electronic Structure,Density of States,Doping Effect*

Highlights

d-MoC(001) surfaces were modified via adsorption and substitution by Ir, Ni, Pd, Pt, Rh and Ru. Iridium showed the highest energetic stability among all tested atomic metals for surface modification

Resumo/Abstract

Transition metal carbides (TMCs) are prominent catalysts and catalyst supports due to their electronic similarity to noble metals. Specifically, molybdenum carbide (δ-MoC) exhibits catalytic properties analogous to those of platinum in methane reforming reactions. In this work, we employed the Vienna Ab initio Simulation Package (VASP) to investigate the effects of the adsorption of metal atoms (Ir, Ni, Pd, Pt, Rh, Ru) on, and their substitution into, the δ-MoC(001) surface. Geometric and energetic parameters were evaluated using DFT-D2 (Grimme) dispersion correction. The adsorption results indicate that the hollow site is the most stable, followed by TopC and TopM sites, respectively. Bridge site proved unstable, converging to TopC positions during geometric optimizations. Furthermore, iridium-adsorbed systems were the most stable across all positions. For the substitution models, no significant surface distortions were observed. Replacing carbon atoms by metal atoms was slightly more stable than substitution of molybdenum atoms. Again, iridium-doped systems showed the highest thermodynamic stability. Band-structure analysis and evaluations of methane activation on the modified surfaces will also be presented.



Adsorption positions of metallic atoms on d-MoC(001) surfaces

Agradecimentos/Acknowledgments

Supported by UnB and SBQ. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001, the Fundação de Apoio à Pesquisa do Distrito Federal (FAP-DF), and the CNPq agency.

Estimation of the Thermodynamic Parameters of Viscous Activation for Esters Present in Biodiesel Using a Theoretically Consistent Method

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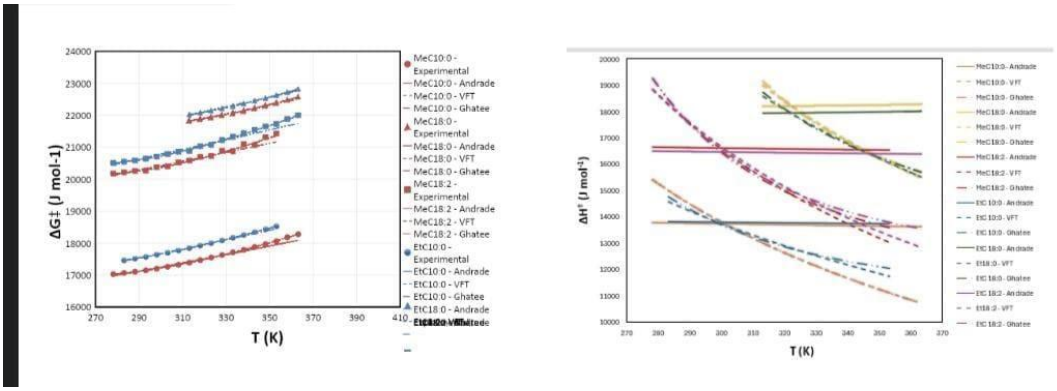
Palavras Chave:*Viscosity,Biodiesel,Eyring's absolute rate equation,Fatty,Thermodynamic Parameters of Viscous Activation*

Highlights

analysis of fatty alkyl esters viscosity using Eyring's absolute rate theory; integration of experimental data with consistent modeling; support for biodiesel process design and simulation.

Resumo/Abstract

Growing environmental concerns, as well as global decarbonization goals, have encouraged the use of renewable fuels, such as biodiesel, whose viscosity is a key parameter for quality control, biofuel performance and production process design. Therefore, it is important to understand and have available models capable of predicting their behavior. In this sense, this work aims to estimate the thermodynamic parameters of viscous activation (ΔG‡, ΔH‡, ΔS‡ and ΔCp‡) of methyl and ethyl esters of fatty acids — the main constituents of biodiesel — through the application of Eyring's absolute rate equation by using a theoretically consistent method. Experimental viscosity and density data available in the literature were compiled and fitted to selected models: Andrade, Vogel-Fulcher-Tammann and Ghatee for viscosity, and the modified-Rackett equation for density, obtaining excellent correlation between experimental and calculated values for most of the models used. Thermodynamic analysis revealed an increase in ΔG‡ and ΔCp‡, as well a decrease in ΔH‡ and ΔS‡ with temperature, behavior analogous to that observed for n-alkanes, indicating that viscous flow is governed by molecular geometry and free volume effects.These results provide a theoretical basis for understanding the viscous behavior of biodiesel components and contribute to the development of predictive models aimed at optimizing fuel processes and formulation. 1)SANTOS, L. J.; ESPINOZA-VELASQUEZ, L. A.; COUTINHO, J. A. P.; MONTEIRO, S. Theoretically consistent calculation of viscous activation parameters through the Eyring equation and their interpretation. Fluid Phase Equilibria, n. 522, p. 112774, 2020. https://doi.org/10.1016/j.fluid.2020.112774. 2)EYRING, H. Viscosity, plasticity, and diffusion as examples of absolute reaction rates. The Journal of Chemical Physics, v. 4, n. 4, p. 283-291, 1936. DOI: https://doi.org/10.1063/1.1749836.



Graphs do ΔG‡ and ΔH‡ and ΔS‡ versus temperature of methyl and ethyl esthers

Agradecimentos/Acknowledgments

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Estudo computacional de complexos de inclusão canabinoide–ciclodextrina via metodologia ONIOM

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Palavras Chave:*canabinoides, ciclodextrinas, ONIOM, modelagem molecular, inclusão*

Highlights

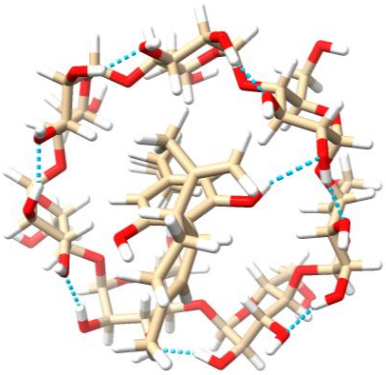
Metodologia ONIOM aplicada a sistemas hospedeiro–hóspede;
Avaliação termodinâmica de complexos canabinoide–CD;
Inclusão molecular visando melhoria de biodisponibilidade.

Resumo/Abstract

Diversos estudos relatam o elevado potencial terapêutico de compostos bioativos derivados da*Cannabis*, associado às suas propriedades antioxidantes, anti-inflamatórias, antibacterianas e neuroprotetoras. Entretanto, a elevada lipofilicidade dessas moléculas compromete a solubilidade em meio aquoso, reduzindo a biodisponibilidade e a eficácia farmacológica por via oral. Nesse contexto, ciclodextrinas (CDs) são amplamente empregadas em sistemas de liberação controlada, promovendo aumento de solubilidade e estabilidade em meios biológicos.

Este trabalho investigou, por modelagem molecular, a formação de complexos de inclusão entre os canabinoides canabidiol (CBD) e canabiciclol (CBCL) com β- e γ-ciclodextrinas, utilizando a metodologia ONIOM. As geometrias foram otimizadas e frequências vibracionais calculadas considerando o complexo como sistema real e o canabinoide como sistema modelo. Para a camada de alto nível, empregaram-se os funcionais M06-2X e ωB97XD com bases 6-31G(d,p) e def2svp, enquanto a camada de menor nível foi descrita pelos métodos semiempíricos AM1, PM3 e PM7. Foram avaliadas duas orientações de inclusão para cada canabinoide, totalizando 98 estruturas otimizadas.

As análises estruturais incluíram o cálculo do RMSD das CDs antes e após a inclusão, a contagem de ligações de hidrogênio e a análise do gradiente de densidade reduzido (RDG), permitindo a caracterização das interações não covalentes responsáveis pela estabilização dos complexos. A análise termodinâmica resultou em $\Delta G = -9{,}4496$ kcal·mol^{-1} a 30 °C para ONIOM(M06-2X/6-31G(d,p):PM3), evidenciando um processo espontâneo e energeticamente favorável. Os resultados confirmam a eficiência da metodologia ONIOM na descrição estrutural e energética dos complexos CD–canabinoide. A pesquisa em questão segue em andamento. Vasquez et al., JPCB (2023); Chung et al., Chem Rev (2015); Park et al., Pharmaceutics (2023).



Complexo BCD–CBD otimizado por ONIOM(M06-2X/def2SVP:PM3); ligações de H em azul.

Agradecimentos/Acknowledgments

Os autores agradecem à CAPES, ao CNPq e à FAPERJ pelo apoio financeiro, e ao CENAPAD São Paulo e LNCC pela infraestrutura computacional disponibilizada para o desenvolvimento deste trabalho.

Estudo Computacional do Mecanismo da Reação de Passerini e da Formação Competitiva de Formamidas

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Palavras Chave:*Reação de Passerini,Quimica verde,Química computacional*

Highlights

Computational study of Passerini reaction

Resumo/Abstract

A reação de Passerini é uma das transformações multicomponentes mais versáteis da química orgânica contemporânea, permitindo a formação simultânea de ligações C–C e C–N a partir de reagentes simples e em condições geralmente brandas. Em 2022, Martinho e colaboradores, descreveram uma variante sustentável desta reação utilizando ácido oxálico sob aquecimento por micro-ondas, levando diretamente à formação de **α**-hidroxi-amidas por um processo subsequente de descarboxilação/descarbonilação do aduto de Passerini. Além da rota principal, os autores observaram a ocorrência de uma reação competitiva que leva à formação de formamidas, cujas origens mecanísticas permanecem pouco compreendidas.
Este trabalho investigou teoricamente o mecanismo detalhado da reação de Passerini com ácido oxálico, incluindo a formação do produto desejado e da via paralela que gera formamidas. Mapeou-se os principais intermediários, complexos de entrada e saída e os estados de transição envolvidos em ambas as rotas, utilizando a Teoria do Funcional da Densidade (DFT) no nível M06-2X/def2-SVP. As energias eletrônicas foram refinadas com o método DLPNO-CCSD(T), e correções termoquímicas foram incluídas com o modelo quase-harmônico de Grimme.

Estudo da descoloração e degradação do corante vermelho Bezaktiv S-Matrix 150 utilizando solução de Fenton em diferentes concentrações de H2O2.

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Palavras Chave:*corante,,vermelho bezaktiv S-matrix 150,descoloração,degradação,Fenton*

Highlights

The efficiency of decolorization and degradation of the red Bezaktiv S-Matrix 150 dye by oxidation with Fenton in different concentrations of H_2O_2 and temperatures were evaluated.

Resumo/Abstract

Um dos objetivos do desenvolvimento sustentável (ODS) é melhorar a qualidade das águas reduzindo a poluição, eliminando dejetos e melhorando os tratamentos, para termos um consumo e produção responsável. Assim, para contribuir com os estudos nessa área, neste trabalho foi estudado a degradação do corante vermelho Bezaktiv S-Matrix 150, utilizado em processos de tingimento na indústria têxtil, pela oxidação com Fenton em diferentes concentrações de H_2O_2 (3%, 5%, 10% e 15%) e temperaturas (30°C, 40°C, 50°C e 60°C). Foi preparada solução de corante na concentração de 0,04 gL^{-1} e solução de Fenton ($H_2O_2/FeSO_4$) com 0,225g de $FeSO_4$ em 100mL de diferentes concentrações de H_2O_2, ajustando o pH para 2 com H_2SO_4. Foram transferidas para uma cubeta de quartzo termostatizada, 3000 µL da solução de corante e 200 µL da solução de Fenton. Leituras da absorbância no comprimento de onda máximo do corante (λ_{max}= 520nm) foram realizadas em intervalos de 2 minutos, durante 40 minutos. Os experimentos foram realizados em duplicatas, e a eficiência de descoloração e degradação da solução do corante foi determinada. As eficiências com diferentes concentrações de peróxidos H_2O_2 e temperaturas (30°C, 40°C, 50°C e 60°C) foram respectivamente: H_2O_2 3% (97%, 98%, 99% e 96%); H_2O_2 5% (13%, 38%, 76% e 94%); H_2O_2 10% (25%, 93%, 93% e 95%); H_2O_2 15% (27%, 44%, 75% e 64%). A**Figura 1**mostra o decaimento da absorbância para a solução de Fenton com H_2O_2 3%. Para otimizar o processo foi avaliado a variação na quantidade de solução de Fenton adicionada a cubeta, mantendo a mesma concentração de corante (0,04gL^{-1}) 50ºC e H_2O_2 3% cujos resultados foram respectivamente: 200 µL (99%), 100 µL (98%), 50 µL (98%),25 µL (95%),12,5 µL (88%),6,2 µL (66%) e 3µL (38%), Nas condições experimentais estudadas da oxidação do corante vermelho Bezaktiv S-Matrix 150 com as diferentes soluções de Fenton, o melhor resultado foi obtido com 200 µL de H_2O_2 3%, 50ºC e 0,04g/L de corante com eficiência de 99% de degradação.

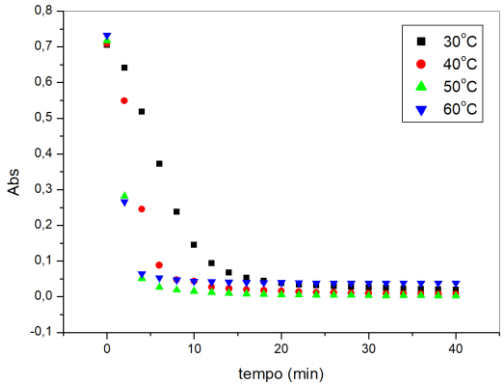


Figura 1 – Decaimento da absorbância vs tempo em diferentes temperaturas com Fenton/H2O2 3%.

Agradecimentos/Acknowledgments

Ao PIBIC/CNPq, CAPES, FAPESC, CLAIMS do Departamento de Química da FURB e ao PPGQ/FURB.

Estudo do comportamento reológico de soluções aquosas de PVA por viscosimetria: efeitos da concentração, temperatura e adição de butanol

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Palavras Chave:*Viscosimetria,PVA,Butanol,Temperatura,hidrogéis*

Highlights

Propriedades reológicas de soluções de PVA com potencial aplicação em hidrogéis Variações do meio modulam o comportamento reológico do PVA.

Resumo/Abstract

O poli(álcool vinílico) (PVA), sintetizado em 1924 por Hermann via hidrólise do poli(acetato de vinila), é amplamente estudado et al, devido às suas propriedades hidrofílicas e aplicações tecnológicas[Hermann, W. O, et al, 1927; Huang, L, et al 2023]. A viscosimetria de soluções poliméricas diluídas é uma técnica sensível para investigar interações polímero–polímero e polímero–solvente, bem como alterações estruturais induzidas por variáveis externas [Brandrup, J et al, 1999; Matsuyama, K, et al, 2017]. O trabalho, avaliou o comportamento reológico de soluções aquosas de PVA por viscosimetria de Ostwald, investigando os efeitos da concentração, da temperatura e da adição de butanol como cosoluto. A solução estoque de PVA 1% (m/v) apresentou formação de gel, atribuída às fortes ligações de hidrogênio entre as cadeias poliméricas e a água. As soluções diluídas entre 0,2 e 1,0% (m/v) apresentaram aumento proporcional dos tempos de escoamento com a concentração, indicando o entrelaçamento progressivo das cadeias. A viscosidade relativa exibiu comportamento linear, permitindo a determinação da viscosidade intrínseca por extrapolação gráfica, resultando em [η] = 0,620 g/dL (R^2 = 0,992).O aumento da temperatura promoveu redução consistente da viscosidade, associada à maior mobilidade molecular e à ruptura parcial das ligações de hidrogênio, evidenciando a termossensibilidade do sistema. Para o estudo com butanol, utilizou-se PVA 0,6% (m/v), com adição de volumes crescentes de butanol (0,2 a 0,8 mL). Observou-se aumento progressivo dos tempos de escoamento em relação ao controle, indicando que o butanol modula a viscosidade por meio de interações hidrofóbicas e reorganização da solvatação das cadeias poliméricas. Os resultados demonstram que temperatura e cossolvente influenciam significativamente a reologia de soluções aquosas de PVA, destacando o potencial do controle viscosimétrico para aplicações em hidrogéis, revestimentos e sistemas de liberação controlada.

Agradecimentos/Acknowledgments

À Universidade Federal do Espírito Santo (UFES) pelo apoio institucional, infraestrutura laboratorial e incentivo à pesquisa científica.

Experimental and theoretical investigation on selegiline inclusion using cyclodextrins.

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Palavras Chave:*Cyclodextrins,Seligiline,Supramolecular Chemistry,ITC,Molecular Dynamics*

Highlights

Carboxymethyl-β-cyclodextrin promotes the strongest host–guest interaction with selegiline. Experimental and theoretical data support the supramolecular complex structure.

Resumo/Abstract

Cyclodextrins (CDs) are widely employed as host molecules to improve the physicochemical and biopharmaceutical properties of drugs through the formation of inclusion complexes, particularly when low solubility or limited bioavailability restrict therapeutic performance. In this work, the supramolecular interaction between selegiline hydrochloride (SEL), an antiparkinsonian drug with low oral bioavailability, and native CDs (α-, β- and γ-CD), as well as carboxymethyl-β-cyclodextrin (CM-βCD), was investigated using experimental and theoretical approaches. Isothermal titration calorimetry (ITC) revealed negligible affinity between SEL and α- or γ-CD, whereas a spontaneous interaction was observed for β-CD, with equilibrium constant (K) of 525 and standard Gibbs free energy change (ΔG°) at −15.6 kJ.mol^{-1} at 298.15 K, due to the |TΔS°| > |ΔH°| the process was entropic driven. A markedly stronger association was obtained for CM-βCD with SEL (K about 3300) and ΔG° value close to −20 kJ mol^{-1}, for the temperatures from 298.15 to 328.15 K. These data reflect the combined contribution of hydrophobic effects and electrostatic interactions between the anionic host and the cationic drug. In order to corroborate the molecular ratio obtained from ITC (3:1 host-guest), molecular dynamics simulations performed with the Gromacs-2024 package aimed to evaluate the formation and structure of the inclusion complex between SEL and CM-βCD. At a certain stage of the simulation, the complex is formed (Figure 1), and subsequently the interaction between CM-βCD and SEL occurs inside the cavity. The ^{1}H/^{1}H 2D ROESY NMR experiments confirmed deep inclusion of SEL into the CM-βCD cavity. Overall, these results emphasize the effectiveness of CD chemical modification in strengthening host-guest interactions and highlight the potential of CM-βCD-based systems to enhance the biopharmaceutical performance of SEL.

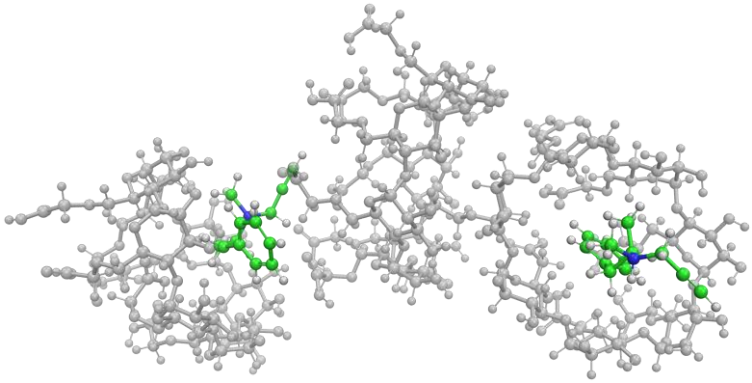


Figure 1. Supramolecular structure of CM-βCD:SEL inclusion complex.

Agradecimentos/Acknowledgments

This work was supported by FAPEMIG (grant numbers APQ-04537-22, RED-00045-23, APQ-00144-24, and APD-00076-25). CNPq (grant number 303311/2024-0), Instituto Nacional de Ciência e Tenologia - Nanobiofar (INCT Nanobiofar), and CAPES.

Foaming of pre-salt light crude oils: Impact of a water-soluble foaming surfactant used in EOR

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Palavras Chave:*foam,crude oil,surfactant,enhanced oil recovery,anti-foaming,Foam,Crude oil,Surfactant,Enhanced Oil Recovery,Anti-foaming*

Highlights

Cocamidopropyl hydroxysultaine (CAHS), a FAWAG/EOR foaming agent, suppresses pre-salt crude-oil foams and changes antifoam efficiency.

Resumo/Abstract

Foam control in Brazilian pre-salt production has become increasingly challenging due to high gas-to-oil ratios and the sensitivity of topside facilities to oil-based foams. In oil-gas separation, pressure reduction releases dissolved gas and can generate stable foams that reduce processing capacity and separation efficiency and may pose safety risks. Although antifoams are routinely applied, the impact of back-produced chemicals on crude-oil foaming and chemical compatibility remains poorly understood. This is especially relevant for Foam-Assisted Water Alternating Gas (FAWAG) in Enhanced Oil Recovery (EOR), which requires water-soluble foaming surfactants that may be back-produced with the fluids. For example, our recent study showed that residual foaming surfactants, even at low ppm levels, can affect water-oil separation in produced fluids, reinforcing the need to assess their broader topside impacts. Here we report preliminary observations for a pre-salt light crude oil and cocamidopropyl hydroxysultaine (CAHS), a water-soluble zwitterionic surfactant widely studied as an aqueous foaming agent. Crude-oil foaming was measured in a Bikerman-type column (N_2 bubbling) using foam height and collapse time, with and without solvent dilution to reduce viscosity. At ambient conditions, the crude showed low foaming tendency, consistent with wax-driven viscosity increase. When viscosity was reduced, the same crude oil produced reproducible foam volumes. CAHS addition (up to 5000 ppm) decreased foam generation and stability, suggesting that interfacial/dispersion effects can dominate in this regime. Antifoam performance differed between crude-oil foams and reference aqueous foams and changed in the presence of CAHS, indicating potential formulation/compatibility effects relevant to field chemical programs. These results highlight the need to monitor FAWAG-surfactant back-production and evaluate chemical compatibility for foam control in pre-salt topside operations.

Agradecimentos/Acknowledgments

This work was supported by Shell Brazil through the R&D N° 23016-9 at PUC-Rio and the strategic importance given by ANP through R&D levy regulation. A.P.G. thanks scholarships from Brazilian agencies FAPERJ (204.241/2024) and CNPq (310713/2025-0).

Formation of self-aggregated systems composed of lecithin, sodium deoxycholate, and cellulose nanofibrils

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Palavras Chave:*Lecithin,Sodium deoxycholate,Cellulose nanofibrils,Rheology,SAXS*

Highlights

Self-assembling systems of lecithin, sodium deoxycholate, and cellulose nanofibrils were developed. It was observed that CNF promotes structuring, colloidal stability and increased viscoelasticity.

Resumo/Abstract

Lecithin is a mixture of phospholipids, widely used in the food industry as a thickener and in the pharmaceutical and cosmetic industries for encapsulating substances[1]. Sodium deoxycholate (NaDC) is a bile salt used for localized fat reduction and drug delivery systems[2]. Cellulose nanofibrils (CNF) are thin, long, and flexible fibers with high mechanical strength and a large surface area, used in packaging, reinforcement, and controlled-release systems[3]. In this work, self-assembling systems composed of lecithin, NaDC in three proportions (0.5, 0.8, and 1 mol/mol), and CNF were developed. The systems were prepared from stock solutions of 200 mM lecithin and 100 mM NaDC in methanol. Lecithin/NaDC mixtures were stirred for 1 h and incubated at 35 °C until complete solvent evaporation. After drying, 10 ml of distilled water was added to systems without CNF, while for systems with CNF, 4.8 ml of the dispersion was added and the remaining volume completed with distilled water to reach 10 ml. The addition of CNF to NaDC systems promoted structural changes compared to systems without CNF. Rheological analyses demonstrate increased viscoelastic character, with higher G' moduli than G' moduli, especially the 100 mM system. This system also showed higher apparent viscosity values; CNF addition promoted an increase from $5x10^{-2}$ to 3305 Pa.s, indicating greater structuring. SAXS analyses showed various structures for systems without CNF, with different diameters, while those with CNF predominantly formed elongated structures (cylindrical micelles). The zeta potential values showed the stability of the systems, with magnitudes above 20 mV, especially for the 80 mM system, where CNF increased values from -29.3 to -54.3.

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From Biomass to Adsorbent: The Role of Thermal Stability in Eucalyptus Coal Production

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Palavras Chave:*kinetic of thermal decomposition, artificial neural network, complex and heterogeneous thermal decomposition process*

Highlights

Thermal stability of eucalyptus-derived coal assessed via TG; Multistage thermal decomposition; Conversion-dependent activation energy revealing progressive stabilization

Resumo/Abstract

This study investigates the role of thermal stability after the transformation of eucalyptus biomass into a functional adsorbent for environmental applications. The thermal stability of coal obtained from eucalyptus (Eucalyptus globulus Labill) was evaluated through thermogravimetric analysis under different heating rates to assess its degradation behavior and kinetic parameters. The kinetic study of the thermal degradation of this charcoal was performed based on thermogravimetric (TG) curves in air (50 mL min^{-1}) at heating rates of 12, 14, and 16°C min^{-1} from 30 to 850°C. The TG curves revealed that the decomposition process occurs mainly between 650 and 830°C, depending on the heating rate, with the degradation shifting to higher temperatures as the rate increases. An artificial neural network was applied, and the results reveal a multistage and heterogeneous decomposition process, with increasing activation energy, from 72 kJ mol^{-1} (10% of conversion) to 100 kJ mol^{-1} (90% of conversion) indicating the progressive breakdown of more stable carbon structures along the decomposition process. Kinetic modeling highlights the contribution of mechanisms such as Avrami-Erofeev (Am2) characterized by nucleation and growth of active sites in the material surface during decomposition. These findings demonstrate that a refined understanding of thermal stability is essential for controlling the physicochemical properties of the resulting material. Understanding the thermal stability of charcoal is crucial for predicting its performance under operational conditions, particularly in adsorption and regeneration cycles. Thermal behavior directly influences pore structure, surface area, and the availability of active sites. Moreover, it supports process optimization during carbonization, enabling better control of material properties. This knowledge ultimately enhances the efficiency, durability, and reliability of charcoal as an environmental adsorbent.

Agradecimentos/Acknowledgments

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Graphene derived multipurpose materials for organophosphate destruction and byproducts adsorption

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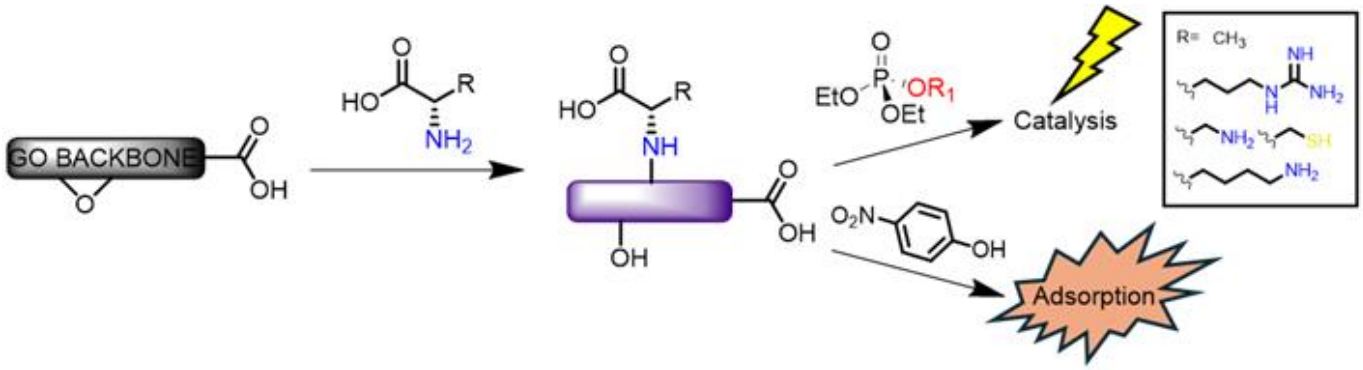
Palavras Chave:*nanochemistry, graphene oxide, functionalization, amino acids, catalysis*

Highlights

Five novel graphene derived materials were synthesized. These materials can enhance dephosphorylation reactions rate and display a strong adsorption towards aromatic compounds

Resumo/Abstract

Organophosphates are a phosphorous compound class widely used as pesticides and chemical warfare agents due to their toxicity. Approaching detoxifying these compounds through catalysis is investigated in this work. Five new graphene oxide (GO) functionalized materials were synthesized via epoxide ring opening reaction. Earlier studies have shown improvement in catalytic performance when utilizing the epoxide opening route compared to the carboxylic route. These studies proposed a general base catalysis mechanism in which the carboxylate abstracts a proton from the nucleophile thus enhancing its nucleophilicity. With that in mind, GO was functionalized with five different amino acids: L-alanine, L-arginine, L-cysteine, L-lysine and L-2,3-diaminopropionic acid. With the functionalizing molecules carrying a carboxylic moiety it is expected a catalytic enhancement when compared to previous studies. Beyond their catalytic performance, these materials demonstrated a high affinity for the adsorption of aromatic compounds. All the materials were characterized by thermal gravimetric analysis, scanning electron microscopy with energy-dispersive X-ray spectroscopy attachment, UV-Vis spectroscopy, Raman spectroscopy, Fourier transformed infra-red spectroscopy and CHNS elemental analysis, confirming their expected chemical nature. The catalytic assessments were done utilizing the organophosphate diethyl-2,4-dinitrophenolphosphate (DEDNPP). All materials exhibited high catalytic activity toward organophosphate degradation, except for L-alanine functionalized GO. Adsorption studies were done utilizing aromatic chromophore compounds such as 2,4-dinitrophenol and 4-nitrophenol and its kinetics/thermodynamic were evaluated through Langmuir's adsorption model. Kinetics fitting for pseudo-second order indicates a strong bond-like interaction between them. In conclusion, these GO derived materials show promising results for the environmental control of organophosphates compounds.



General scheme for GO functionalization and materials applications

Agradecimentos/Acknowledgments

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Heteroestruturas de Ferritas de Zinco com Óxido de Grafeno Reduzido para a Remediação de Contaminante Orgânico

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Palavras Chave:*Método de Co-precipitação, Ferritas de zinco, Fotocatálise,Método de Coprecipitação, Ferritas de zinco, Fotocatálise.,Método de Co-precipitação, Ferritas de zinco, Fotocatálise*

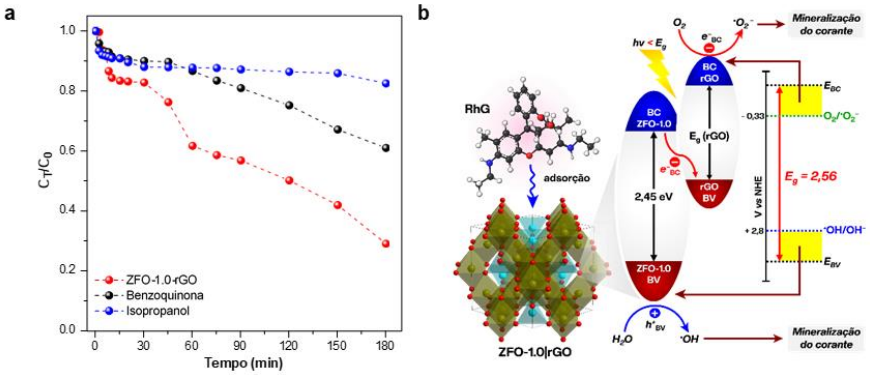
Highlights

Ferritas de zinco foram sintetizadas pelo método de co-precipitação com estrutura tipo espinélio.

As ferritas de zinco exibiram maior fotodegradação da rodamina 6G sob irradiação de luz visível.

Resumo/Abstract

Ferritas de zinco ($ZnFe_2O_4$) tem emergido como semicondutores aplicados em fotocatálise heterogênea para o tratamento de águas residuais. No entanto, um dos problemas associados às ferritas de zinco é a recombinação dos pares elétrons-buraco nos sítios catalíticos do material. A formação de heterojunções, estruturas que promovem a separação eficiente dos portadores de carga, é uma dessas estratégias. Nesse sentido, o presente trabalho busca investigar a atividade fotocatalítica de heterojunções de ferritas de zinco (ZFO) e óxido de grafeno (GO) reduzido $Zn_xFe_{3-x}O_4$/rGO (onde x varia entre 0,6 e 1,2) como potenciais fotocatalisadores na degradação de contaminate orgânico, como a Rodamina 6G (RhG). Os pós de ZFO foram sintetizados pelo método de co-precipitação a partir de soluções precursoras contendo sais de Zn^{2+} e Fe^{3+}, e calcinados a 700ºC por 4 horas em atmosfera de N_2. O GO foi obtido pelo método de Hummer via oxidação do grafite. As heterojunções foram obtidas a partir dos precursores sólidos pela síntese de refluxo a 100 ºC durante 12 h, promovendo a redução térmica do GO, que é convertido em óxido de grafeno reduzido (rGO), resultando na heteroestrutura. A análise estrutural, por difração de raios X, indicou a formação da fase $ZnFe_2O_4$ de estrutura tipo espinélio normal de simetria cúbica e grupo espacial*Fd-3m*.A análise por microscopia eletrônica de varredura das heterojunções apresentou as características morfológicas de ambos os precursores. Os espectros Raman identificaram os modos vibracionais associados às ferritas, e modos relacionados à organização das camadas de GO. Os valores de*band gap*das heteroestruturas apresentaram valores entre 2,39 e 2,59 eV. O estudo cinético dos pós de $Zn_xFe_{3-x}O_4$/rGO foi realizado sob luz visível, em solução de RhG, considerando a variação do pH em meio ácido (4), neutro (7) e básico (10). A estequiometria $ZnFe_2O_4$/rGO apresentou a maior taxa de fotodegradação de 70,9% em pH ácido ao final de 180 minutos.



a) Cinética de degradação, b) Representação do processo fotocatalítico para o ZFO- 1.0/rGO.

Agradecimentos/Acknowledgments

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High Internal Phase Emulsions (HIPEs) stabilized by particles formed by the complexation of biopolymers

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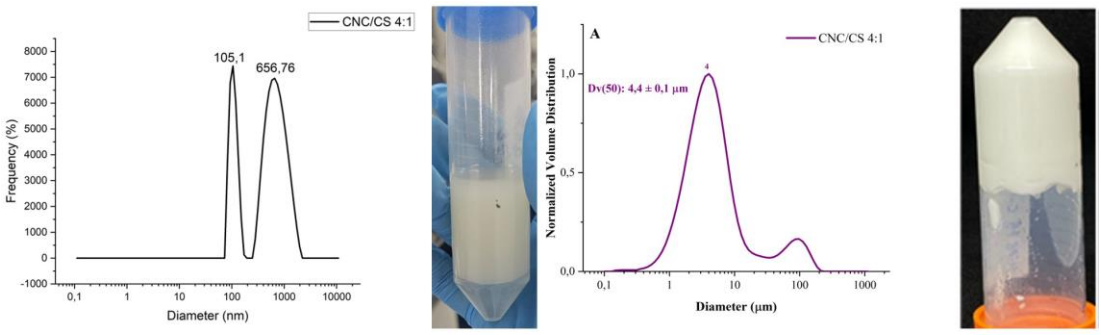
Palavras Chave:*chitosan,CNC,sustainability,food,cellulose*

Highlights

Complexation of chitosan and cellulose forms tunable particles
Biopolymeric particles stabilize O/W high internal phase emulsions (HIPEs)
O/W HIPE present rheological property for use in food industry

Resumo/Abstract

High internal phase emulsions (HIPEs) exhibit rheological properties similar to saturated fats used in the food industry. This study focused on developing particles by complexing chitosan (CS) with cellulose nanocrystals (CNC) to stabilize oil-in-water (O/W) HIPEs via the Pickering mechanism. In the first stage, physicochemical, structural, and functional properties of particles obtained by different complexation methods (direct mixing or dropwise addition) were investigated. Characterization was performed using optical microscopy, laser diffraction, dynamic light scattering (DLS), and zeta potential analysis. Results showed that particle can be tuned from hundreds of nanometers to several micrometers depending on the preparation method. For instance, dropwise addition (0.015 mL) of CNC dispersion into CS solution produced two populations of 105.1 and 656.76 nm (Figure 1a), whereas inverted addition (CS into CNC) led to large, non-dispersible aggregates. Direct mixing generated particles with a main population of 4.4 µm (Figure 1c). Despite maintaining the same CNC:CS ratio (4:1), particles from dropwise addition exhibited negative zeta potential (-60 mV), while direct mixing yielded positively charged particles (+50 mV). In the second stage, these particles were applied to prepare O/W HIPEs containing 75% oil. The smallest particles (Figure 1a) failed to stabilize the emulsion, which separated immediately (Figure 1b). Conversely, the micrometric, positively charged particles obtained by direct mixing enabled HIPE formation (Figure 1d). The emulsions were further characterized by microscopy, laser diffraction, and rheology. Results confirmed their potential as fat substitutes in food applications, though stability was limited to 48 h. In conclusion, particle and zeta potential of CS–CNC complexes can be controlled by the addition method, directly influencing HIPE properties and offering a pathway to optimize them for industrial use.



a) DLS size by dropwise, b) emulsion by dropwise, c) LD size by mixture, d) HIPEs by mixture

Agradecimentos/Acknowledgments

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Hydrogen Bonding and Counterion Effects on the SN2 vs E2 Reactions in Nucleophilic Fluorination of Secondary Alkyl Substrates

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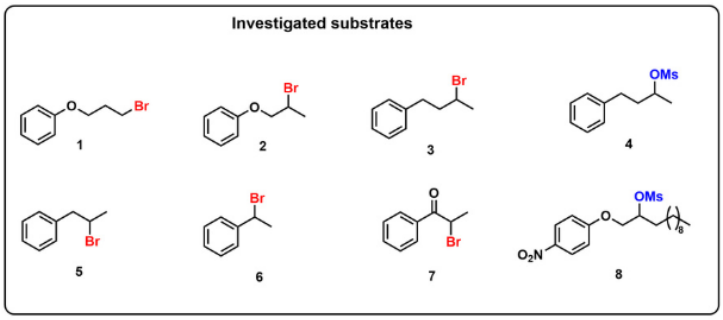
Palavras Chave:*hydrogen bonding, solvent effects, late-stage fluorination, phase-transfer catalysis, theoretical calculations, ion-pairing.*

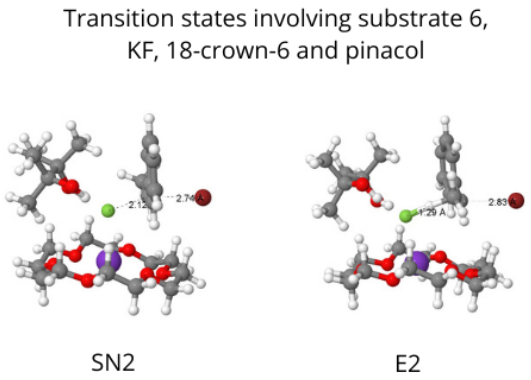
Highlights

DLPNO-CCSD(T) barries quantify SN2/E2 competition across alkyl substrates
Pinacol/TBOH-F3 H-bonding and K^+-18C6 ion pairing drive selectivity
Mesylates lead to less E2 than bromides
TBAF is more reactive

Resumo/Abstract

Synthesizing secondary alkyl fluorides through nucleophilic substitution is challenging because of significant competition from E2 elimination reactions. This competition is influenced by factors such as the substrate's chemical environment, the counterion, and how the fluoride ion interacts through hydrogen bonding. In this study, we used a combination of theoretical calculations and experimental work to investigate the reactivity and selectivity of eight substrates. Our calculations highlighted the importance of SN2 versus E2 competition under different reaction conditions and chemical environments. Experimentally, we tested potassium fluoride combined with 18-crown-6 and bulky alcohols like pinacol and 2-trifluoromethyl-2-propanol (TBOH-F3) with several alkyl bromides and mesylates. We also assessed tetrabutylammonium fluoride (TBAF) combined with these alcohols. The results showed that potassium fluoride with crown ether and bulky alcohols offered higher selectivity than TBAF with the same alcohols, though TBAF was more reactive. Alkyl mesylates were less likely to yield E2 products, and high fluorination yields were achieved using KF with 18-crown-6 and pinacol in acetonitrile. Additionally, we identified 2-bromo-1-phenylpropane (substrate 5) as particularly difficult to fluorinate. Our work highlights how controlling intermolecular forces close to the reaction center allows better control of reactivity and selectivity of these ionic reactions.





Investigated substrates using theoretical and experimental methods.

Agradecimentos/Acknowledgments

This work was supported by FAPEMIG, CNPq, and CAPES.

IMIDAZOLE FUNCTIONALIZED BIOMATERIALS AIMING THE NEUTRALIZATION OF ORGANOPHOSPHATE-BASED PESTICIDES

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Palavras Chave:*Biomaterials, pesticides, organophosphates, catalysis, imidazole*

Highlights

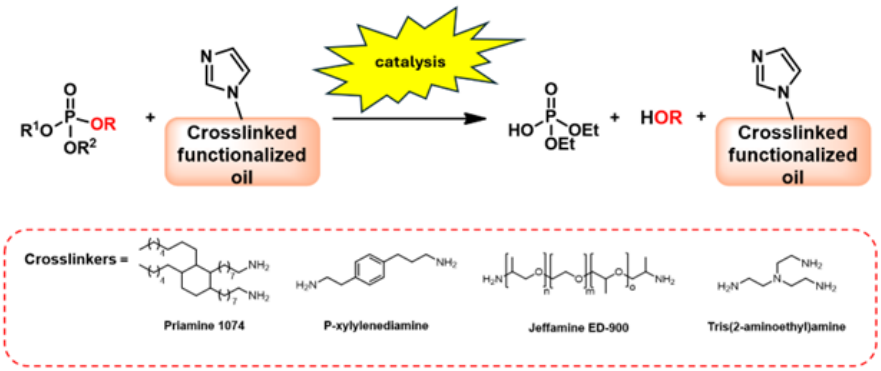
Imidazole-functionalized biomaterials sourced from linseed oil were synthesized aiming new potential catalysts on the degradation of organophosphate-based pesticides.

Resumo/Abstract

With the growing interest in neutralization of organophosphate-based pesticides, the need for new and more efficient ways of catalyzing the degradation of these molecules increased in the last few years. Imidazole has been considered a highly effective catalyst in this process. Biomaterials sourced from linseed oil (LO) and functionalized with imidazole can be great alternatives in this scenario, facilitating the catalyst recovery. Herein, we produced 4 biomaterials derived from imidazole and linseed oil reticulated with Jeffamine ED-900, Priamine 1074, p-xylylenediamine and tris-2-aminoethylamine. These crosslinkers were chosen due to their different chemical properties, such as aromaticity, polarity and size of the carbon chain. By changing crosslinkers, we can investigate how their interaction with the solvent and/or the organophosphate can interfere with the reaction rate. These biomaterials were characterized by several techniques (NMR, TGA, DSC, CHNS, FTIR, MEV, swelling and extractables assays), confirming the functionalization with imidazole and, also, the absence of non-reactant crosslinkers.

The biomaterials were used as nucleophilic catalysts towards the degradation of 2,4-dinitrophenyl diethyl phosphate at, with catalytic increments up to 103-fold under mild condition (25oC, pH 8,5), compared to the spontaneous reaction.

Materials reticulated with aromatic crosslinkers presented higher catalyst potential even with smaller functionalization degrees, indicating that the interaction between the crosslinker and the organophosphate is very important for the increasing of reaction rates. These materials were also tested in recycling studies, and it was observed that the rate constant of the reactions remained similar even after 5 reuses . To summarize, we produced 4 imidazole-functionalized biomaterials that act as catalysts in the degradation of organophosphates and can be easily reused, advancing in the topic of chemical safety regarding pesticides.



Degradation of OPs catalyzed by imidazole-functionalized biomaterials derived from linseed oil.

Agradecimentos/Acknowledgments

UFPR, CAPES, CNPq, L'Oréal UNESCO-ABC, PhosAgro/UNESCO/IUPAC, INCT NanoVida, INCT Nanocarbono e Materiais 2D, INSA, Région Normande, École doctorale Normande de chimie

Immobilization of L-cysteine on a chemically modified cellulose platform derived from rice husks

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Palavras Chave:*cellulosic platform,cysteine immobilization,click-chemistry,thiol-yne reaction,thiol-yne reaction,thiol-yne reaction*

Highlights

Rice husk cellulose was propargylated and used to immobilize L-cysteine via photoinitiated thiol-yne click chemistry, producing a functionalized and thermally stable cellulosic material.

Resumo/Abstract

Global rice production generates large amounts of rice husk residues (CA) that are mainly exploited for their silica content but also contain significant amounts of lignocellulosic material [1]. This polymeric matrix, composed primarily of cellulose, hemicellulose, and lignin, represents a promising renewable resource for the development of functional materials. This work aims to develop a chemically modified cellulose platform derived from CA for molecular immobilization using click chemistry. α-Cellulose was isolated from CA by alkaline extraction and subsequently etherified with propargyl bromide to introduce alkyne functionalities, yielding propargyl-cellulose (PCA). L-cysteine was then used as a model molecule and immobilized onto this platform through a photoinitiated thiol-yne click reaction under green light irradiation, producing cysteine-functionalized cellulose (CAC). Fourier transform infrared spectroscopy (IR) confirmed the introduction of alkyne groups in the modified cellulose by the appearance of the characteristic band at 2113 cm^{-1} attributed to the C≡C bond stretching vibration. After the thiol-yne reaction, additional bands in the 777-844 cm^{-1} region associated with C-S bonds and a band near 1655 cm^{-1} attributed to the amide group of cysteine were observed, indicating successful immobilization on the PCA matrix. Thermogravimetric analysis showed distinct thermal degradation profiles for the materials obtained in each synthesis step, confirming chemical modification of the cellulose platform. The cysteine-functionalized cellulose remained thermally stable up to approximately 200 °C. The results demonstrate that the proposed strategy enables the immobilization of thiol-containing molecules on a cellulose platform derived from agricultural residues and may be extended for the immobilization of more complex molecules. [1] Peralta Y. M.*et al.*, Journal of Environmental Management, v. 370, 2024. https://doi.org/10.1016/j.jenvman.2024.122735

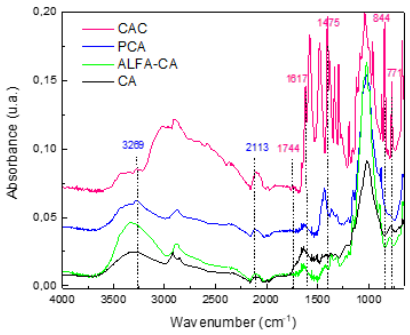


Fig.1A

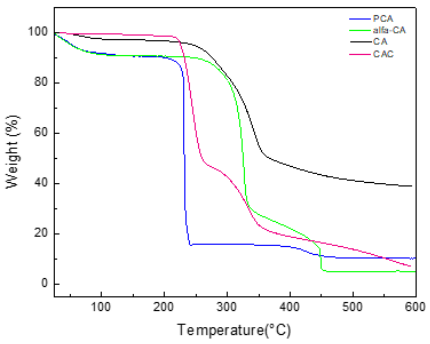


Fig1B

FTIR absorption spectra(1A)and Thermogravimetric curves(1B) for CA, alfa-CA, PCA, and CAC samples.

Agradecimentos/Acknowledgments

authors are thankful to the FAPEMIG, UFU, CAPES, PROPP, and RELAM-UFU.

Influence of Hartree-Fock Fine-Tuning on the Theoretical Description of Natural Dyes from the Brazilian Flora for DSSC Applications

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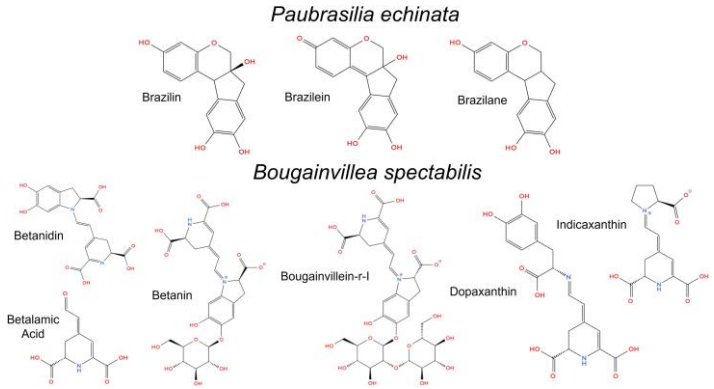
Palavras Chave:*DFT,TD-DFT,Fine-Tuning,Natural Dye,Solar Cell*

Highlights

Conformational screening of natural pigments from Brazilian flora via CREST and GFN2-xTB. Hartree-Fock Exchange fine-tuning in modified B3LYP functional improves the description of excitation energies.

Resumo/Abstract

A theoretical investigation of natural pigments from*Paubrasilia echinata*and*Bougainvillea spectabilis*as potential sensitizers for dye-sensitized solar cells (DSSCs). The methodology employs a multi-step computational protocol with conformational screening using the CREST tool with the GFN2-xTB method under implicit methanol solvation (ALPB model). Structural refinement using Density Functional Theory (DFT) at B3LYP/6-31G(d,p) level. Time-Dependent DFT (TD-DFT) was applied using two complementary strategies to accurately characterize photophysical properties. CAM-B3LYP was used to describe excited states with intramolecular charge transfer (ICT). A systematic fine-tuning of the Hartree-Fock (HF) exchange percentage, ranging from 0.15 to 0.25 in the modified B3LYP functional (modB3LYP) was performed to mitigate self-interaction errors and refine excitation energies. Electronic excitations were analyzed via absorption spectra and Hole-Electron distribution using Multiwfn software. Results indicate that most studied pigments possess absorption profiles in spectrally relevant regions. The molecules obtained satisfactory results in specific photovoltaic parameters, although some structures exhibit Locally Excited (LE) character instead of ICT. The energy levels of the Frontier Molecular Orbitals of some molecules align with the conduction band of titanium dioxide (TiO_2) and the redox potential of the iodide/triiodide (I^-/I_3^-) electrolyte, ensuring conditions for electronic injection and dye regeneration. Electronic density moves from donor groups to anchoring moieties in specific cases. HF fine-tuning protocol is essential for a reliable description, as standard hybrid functionals often fail to capture the nuances of complex electronic systems. Despite limitations, this work establishes methodological foundations for computational screening of sustainable materials, contributing to the development of renewable technologies based on Brazilian flora resources.



Chemical structures of natural pigments from P. echinata and B. spectabilis for TD-DFT analysis.

Agradecimentos/Acknowledgments

The authors thank CAPES, CNPq, FAP-DF, and UnB for funding. Support from the Institute of Chemistry and the LMSC/UnB, LQC/UnB and LEEDMOL/UFG laboratories was essential for the development of this research.

Influence of pH on the antibody–antigen interface: An investigation using constant-pH molecular dynamics

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Palavras Chave:*scFv from M971,Constant-pH,CD22,Molecular Dynamics*

Highlights

CpHMD simulations show that the short linker (scFv-S) increases the stability of the scFv/CD22 interface via His136 protonation, defining a protocol for testing the tumor microenvironment (pH 6.5).

Resumo/Abstract

B-lineage Acute Lymphoblastic Leukemia (B-ALL) has been shown to express the CD22 antigen. This represents a strategic therapeutic target for the development of Chimeric Antigen Receptor-T (CAR-T) cells. The efficacy of this therapy is contingent upon the antigen-recognition domain of the Chimeric Antigen Receptor, the single-chain variable fragment (scFv). It has been demonstrated by preceding studies that the linker length between the heavy (VH) and light (VL) variable domains exerts a significant influence on the affinity of scFv–CD22. Furthermore, ionizable residues have been identified at the scFv/CD22 interface. To investigate how the protonation states of these residues affect interface stability, constant-pH molecular dynamics (CpHMD) simulations at pH 7.4 were performed using the method recently implemented in GROMACS 2021 by Aho et al. (2024). The focus of this study was two scFvs interacting with CD22, differing in linker length and derived from M971 (PDB code 7O52; scFv-S and scFv-L). Preliminary CpHMD results, based on a λ-dynamics analysis, showed that in the scFv-S/CD22 system, CD22 histidine 136 is frequently protonated at both delta and epsilon nitrogens (HIP), whereas in the scFv-L/CD22 system it is predominantly protonated only at delta or epsilon positions (HID/HIE). Principal component analysis (PCA) of the three-dimensional structures indicated greater stabilization of the scFv-S/CD22 system. It is concluded that CpHMD reveals a pH-dependent structural stability of the scFv/CD22 interface, and that the protocol established here will be extended to scFv-S/CD22 and scFv-L/CD22 systems at pH 6.5 to mimic the tumor microenvironment.

Agradecimentos/Acknowledgments

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Programa de Biotecnologia de Recursos Naturais da Universidade Federal do Ceará (Ppgbiotec-UFC)

Intelligent Fault Monitoring of Nonlinear Chemical Dynamics Using an Artificial Immune System Applied to the Brusselator

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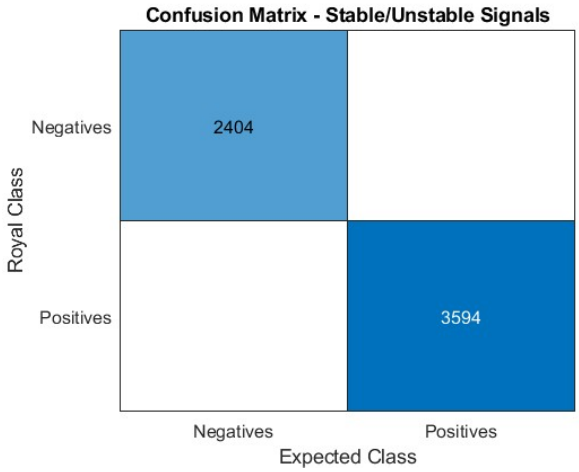
Palavras Chave:*Artificial Immune System,Brusselator,Nonlinear Dynamics,Fault Detection,Chemical Instabilities*

Highlights

Artificial immune systems were applied to monitor nonlinear chemical instabilities.
Brusselator dynamics were classified with high accuracy.
Real-time fault detection was achieved.

Resumo/Abstract

Nonlinear chemical systems operating far from thermodynamic equilibrium often exhibit oscillatory and unstable behaviors that pose significant challenges for monitoring and control. Among such systems, the Brusselator model is a paradigmatic framework for studying autocatalytic reactions, bifurcations, and transitions to instability. In this work, an intelligent fault monitoring system based on an Artificial Immune System (AIS), specifically the Negative Selection Algorithm, is proposed to detect and classify stable and unstable dynamical regimes of the Brusselator. A comprehensive database was generated through numerical simulations of the Brusselator model under different parameter settings, producing time series associated with normal (stable) and faulty (unstable) behaviors. The AIS was trained during an offline censoring phase to construct a set of detectors representing normal operating conditions. In the online monitoring phase, incoming signals were continuously evaluated through self/non-self discrimination to identify deviations from nominal dynamics. The proposed system demonstrated excellent performance in fault detection, achieving an accuracy of 99.83% and perfect classification metrics, including accuracy, sensitivity, precision, specificity, and F1-score equal to 1.00. The processing time remained compatible with real-time monitoring requirements, highlighting the computational efficiency of the approach. These results indicate that artificial immune systems constitute a robust and adaptive framework for monitoring complex nonlinear chemical reactions, offering promising perspectives for applications in chemical reactors, process safety, and intelligent supervision of reactive systems.



Confusion Matrix - Stable/Unstable Signals

Agradecimentos/Acknowledgments

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INTERFACIAL ORGANIZATION AND PHYSICOCHEMICAL CHARACTERIZATION OF SELF-ASSEMBLED COLLOIDAL SYSTEMS CONTAINING ORGANOSELENIUM COMPOUNDS

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Palavras Chave:*Organoselenium compounds, self-assembly, colloidal systems, nanoemulsions, biosurfactants.*

Highlights

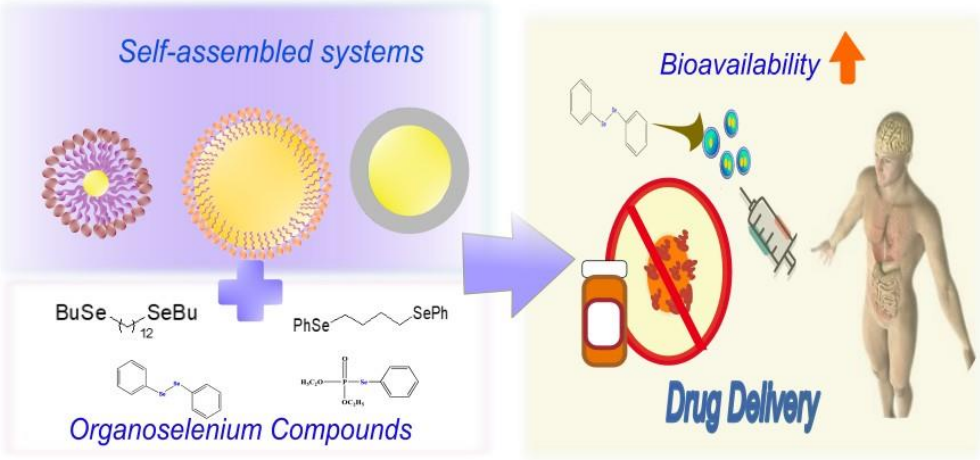
Investigation of self-assembly and interfacial organization in organoselenium-loaded collidal system
Application of biosurfactants in colloidal formulations

Resumo/Abstract

Organoselenium compounds constitute an important class of organochalcogens, extensively studied due to their distinctive physicochemical and pharmacological properties, with potential applications in biomedicine, catalysis, and organic synthesis. However, their high lipophilicity significantly limits solubility in aqueous media, restricting bioavailability and performance in biological environments. From a physical chemistry perspective, controlling intermolecular interactions and self-assembly processes is essential to overcome these limitations.

In this work, different self-assembled systems—micelles, emulsions, nanoemulsions, and nanocapsules—were developed to incorporate novel organoselenium compounds synthesized in our laboratory. The formulations were prepared using classical pharmaceutical excipients as well as innovative systems based on biosurfactants (bioloop), which remain largely unexplored in the context of colloidal self-assembly. Among the investigated systems, nanoemulsions were emphasized due to their kinetic stability, tunable interfacial properties, and relevance as model colloidal systems.

The obtained systems were characterized in terms of average particle size, size distribution, and zeta potential, providing insights into colloidal stability and interfacial charge. UV–Vis and FTIR spectroscopy were employed to investigate molecular interactions between the organoselenium compounds and the nanostructured matrices. Biological studies are currently under planning, with a focus on evaluating oxidant and/or antioxidant activity, aiming to correlate physicochemical parameters with potential biological performance. This study highlights the role of self-assembly and colloidal organization as physicochemical strategies to modulate the properties of organoselenium compounds and expand their applicability.



Enhancement of organoselenium compound bioavailability through self-assembled systems.

Agradecimentos/Acknowledgments

UFSM, CAPES, FAPERGS, CNPq, LABSRAFTO, SMLab, UFPR, GCC, BIOPOl, L'Oréal UNESCO-ABC, PhosAgro/UNESCO/IUPAC, INCT NanoVida, INCT Nanocarbono.

Intramolecular Pnictogen Bonds as Key Determinants for NMR Quantum Computation Parameters

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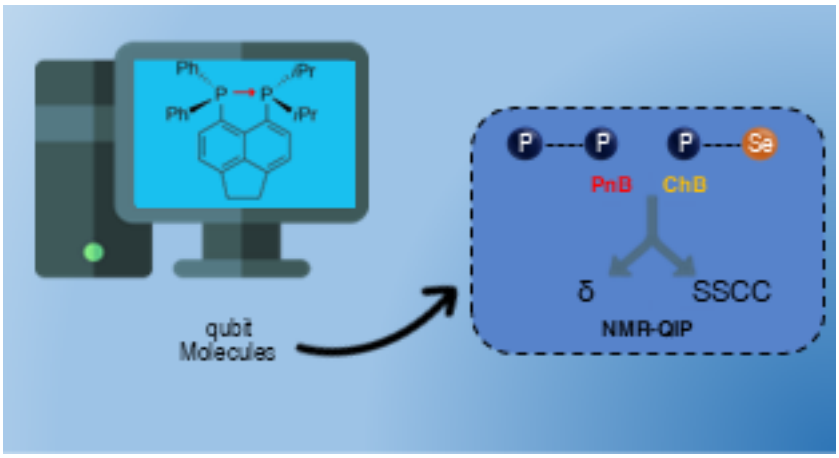
Palavras Chave:*Pnictogen Bonds,NMR Quantum Information Processing,Qubits,Spin-Spin Coupling Constants,DFT Calculations*

Highlights

Stronger PnB enhance NMR parameters, making molecules more suitable for quantum computing. Interaction analyses reveal the covalent nature of intramolecular interactions in potential qubits.

Resumo/Abstract

In nuclear magnetic resonance (NMR) quantum information processing (QIP), the design of molecules capable of fulfilling the DiVincenzo criteria strongly depends on the control of NMR parameters such as chemical shifts (δ) and spin–spin coupling constants (SSCC). Since these parameters are highly sensitive to intramolecular interactions, understanding how specific interactions affect them is essential for rational quantum bits (qubit) design. In this work, four naphthalene and acenaphthene derivatives, were investigated via Density Functional Theory (DFT) to assess their potential as qubits for NMR-QIP. The study focused on the influence of intramolecular interactions, specifically pnictogen bond (PnB), on the NMR properties of P and Se nuclei. To deeply characterize the P-P and P-Se interactions, Atoms-in-Molecules, Natural Bond Orbital, and Energy Decomposition Analysis were employed. These analyses revealed that the interactions are not purely electrostatic, instead, orbital interactions are the dominant stabilizing factor, contributing approximately 70% to the total interaction energy, which indicates a significant covalent character. Furthermore, to explicitly determine the role of PnB strength in QIP suitability, the internuclear distance between phosphorus atoms was systematically modulated. The results established a direct correlation, as the atoms approach and the interaction strengthens, the SSCC values increase significantly, a behavior primarily attributed to the enhancement of the Fermi contact term. Simultaneously, the δ is modulated, leading to greater differentiation between the nuclei. In summary, the findings highlight that the rational design of intramolecular pnictogen interactions serves as a viable strategy to fine-tune magnetic properties, optimizing compounds for advanced applications in quantum computing.



Overview of the work: intramolecular interactions shaping NMR parameters

Agradecimentos/Acknowledgments

The authors are thankful to CAPES, FAPEMIG, CNPq, FINEP, and INCT Defesa. This study was supported by Excellence Project UHK.

Machine Learning, Molecular Dynamics, and QM/MM Free Energy Calculations Reveal the Potential of Repositioned Compounds as 5-HT1A Agonists for ASD.

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Palavras Chave:*ASD,QSAR,QM/MM,ADMET predictions,Virtual screening*

Highlights

Key binding interactions involved Asp246 and Asn516 residues.

Docking validation achieved high accuracy (AUC = 0.823).

ADMET predictions point to ligands with blood-brain permeability

Resumo/Abstract

This study employs an integrated computational approach to identify potential 5-HT_1A receptor agonists for treating Autism Spectrum Disorder (ASD), addressing the critical lack of targeted pharmacological therapies. Focusing on repurposing strategies, we screened the CHEMBL database for compounds containing Piperazine-(1,4R) and 1H-Indole-(3R) scaffolds. The methodology utilized homology modeling to complete the 5-HT1A crystal structure (PDB: 8FYX), followed by rigorous ADMET predictions to prioritize compounds with blood-brain barrier permeability and optimal safety profiles. A molecular docking protocol, validated by an ROC curve (AUC = 0.823), combined with MLR-QSAR modeling to predict pEC_{50} values. The QSAR model demonstrated high statistical robustness (r^2 = 0.847,q^2LOO = 0.670) and strong external predictive power ($r^2_{p}r_{e}d$ = 0.751, CCC = 0.789, MAE=0.350). The top three candidates, PP1, PR1 (Anamorelin), and PR2 (Temsavir), underwent 200 ns Molecular Dynamics simulations and QM/MM-GBSA free energy calculations. All three displayed superior binding stability compared to Buspirone, the standard reference agonist. Binding free energies were computed using the QM/MM-GBSA method with the PM6-DH+ semiempirical Hamiltonian. Temsavir (PR2) displayed the most favorable binding affinity ($\Delta G bi_n di_n g$= −33.61 kcal/mol), driven by significant electronic stabilization (ΔESCF = −22.77 kcal/mol). This significantly outperformed the reference agonist Buspirone ($\Delta G bi_n di_n g$= −14.05 kcal/mol). The study identified crucial stabilizing interactions, specifically π-anion interactions with Asp246 and hydrogen bonds with Asn516, positioning Temsavir as a promising candidate for experimental validation in ASD therapy.

Agradecimentos/Acknowledgments

The authors are thankful to CNPq, CAPES, FAPEMIG Federal University of Lavras and Departament of Chemisty.

Metal-Ligand Interactions in Iron (II) Photosensitizers

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Palavras Chave:*iron(II) photosensitizers, DFT and CCSD(T) calculations, electronic and molecular properties, local energy decomposition analysis,iron(II) photosensitizers,DFT and CCSD(T) calculations,electronic and molecular properties,local energy decomposition analysis*

Highlights

Substituent effects (-H, -COOH, -OMe) on Fe - ligand bonding in Fe(II) photosensitizers investigated by DFT and DLPNO-CCSD(T) local energy decomposition (LED)

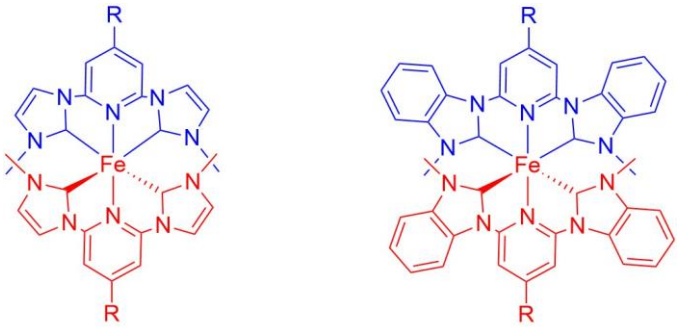
Resumo/Abstract

This work investigates the effect of ligand substitution (-H, -COOH, -OMe) on metal-ligand interactions and MLCT photophysics in the Fe(II) photosensitizers $[Fe(pbmi)_2]^{2+}$ and $[Fe(pbmbi)_2]^{2+}$ (Figure 1). Geometries were optimized at the DFT/PBE-D3(BJ)/def2-TZVP level, and Local Energy Decomposition (LED) analyses were performed using DLPNO-CCSD(T)/def2-TZVP to quantify electrostatic, exchange, correlation and dispersion contributions. Calculations were carried out with ORCA.

At the DFT/PBE-D3(BJ)/def2-TZVP level, we find the HOMO--LUMO gap ordering: OMe > H > COOH for both complexes (e.g. ≈ 2.46, 2.25, 1.96 eV for the*pbmi*series), consistent with Hammett parameters and the donor/acceptor character of the substituents. Geometric changes upon substitution are small (hundreds of 0.01 Å in bond lengths and < 1° in bond angles) compared to the parent structures. Local Energy Decomposition at the DLPNO-CCSD(T)/def2-TZVP level shows that interaction energies vary with the substituent and do not strictly track the HOMO-LUMO gaps, pointing to a nontrivial balance between electrostatic, exchange, correlation and dispersion components.

Considering the experimentally reported MLCT lifetimes (≈ 10 ps for $[Fe(pbmi)_2]^{2+}$ and ≈ 16 ps for $[Fe(pbmbi)_2]^{2+}$ with the -H substituent), a clear correlation emerges between the metal–ligand interaction energy and MLCT lifetime. For the*pbmi*complex with the -H substituent, a stronger Fe–L interaction energy ΔEi_{nt} = -232.60 kcal/mol is associated with a shorter MLCT lifetime (≈ 10 ps), whereas for the*pbmbi*analogue, a slightly weaker interaction energy ΔEi_{nt} = -231.35 kcal/mol corresponds to a longer MLCT lifetime (≈ 16 ps). This trend suggests that the greater (or lower) the Fe–L interaction energy, the shorter (or longer) the MLCT lifetime, indicating that weaker metal–ligand interactions may favor MLCT state stabilization and slower decay.

This analysis highlights molecular-level trends relevant to extending MLCT lifetimes and supports the rational design of earth-abundant iron photosensitizers for photocatalysis and solar-energy applications. Results will be expanded with systematic benchmarks and solvent models.



LED fragmentation of (A) [Fe(pbmi)2]^2+ and (B) [Fe(pbmbi)2]^{2+}}. Frag. 1 (red) and Frag. 2 (blue)

Agradecimentos/Acknowledgments

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Modelagem molecular da interação do Canabinol, Canabiciclol e derivados com protofilamentos da beta-amiloide

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Palavras Chave:*Alzheimer,Canabinoides,In sílico,Data mining,Inteligência Artificial*

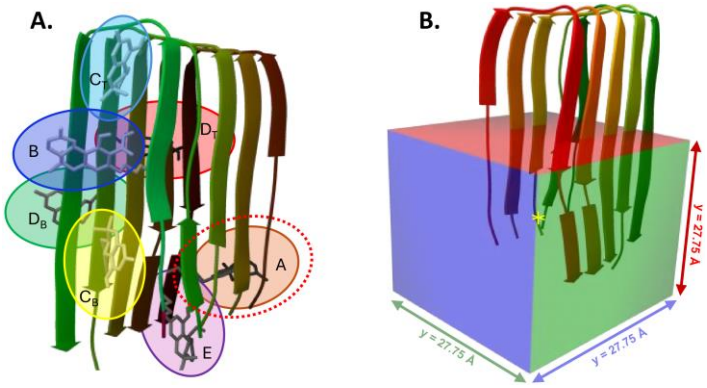
Highlights

Heatmap and PCA analysis revealed strong ligand correlations;
Highly hydrophobic ligands forms stable ligand-receptor complexes;
Carbonyl substitutions alter LUMO distribution and electron density.

Resumo/Abstract

A doença de Alzheimer (DA) é uma doença neurodegenerativa responsável pelo maior número de casos globais de demência que ainda carece de tratamentos eficazes. Um de seus marcadores mais bem estabelecidos na literatura é o acúmulo de placas de β-amiloide (Aβ). Embora não seja clara a contribuição destas para a progressão da DA, evidências como a capacidade destas placas em induzir um quadro de inflamação cerebral e apoptose neuronal as apontam como cruciais para o desenvolvimento da DA. O objetivo deste trabalho foi estudar, por meio de estudos in sílico e técnicas de data mining, as interações dos canabinóides minoritários (CMs) canabinol (CBN), canabiciclol (CBL) e seus derivados, com os protofilamentos de uma conformação conhecida da Aβ (código PDB 2BEG). Com este objetivo, preparou-se das estruturas geométricas dos CMs estudados e do receptor biológico. As conformações de menor energia dos CMs foram obtidas por meio de cálculos de estrutura eletrônica (EE) utilizando a teoria do funcional de densidade com o funcional híbrido M06-2x e a função de base aug-cc-pVDZ, com modelo de solvatação implícita SMD com água como solvente. Foram determinados os índices de reatividade dessas moléculas, as interações não covalentes e índices de Fukui. Uma avaliação no perfil farmacofórico dos CMs usando os dados ADMET e de EE foi feita por meio da aplicação de data mining e inteligência artificial usando algoritmos de heatmap e PCA. Por fim, foi realizado um estudo de docking entre o receptor e as conformações resultantes com as cargas atômicas obtidas pelo método quântico ChelpG.

Observamos que mudanças estruturais afetam significativamente a distribuição dos orbitais LUMO e na densidade eletrônica dos ligantes. Os estudos de docking revelaram que ligantes com maior caráter hidrofóbico tendem a formar complexos mais estáveis com o receptor. Esses resultados auxiliarão na busca por moléculas com maior afinidade pela Aβ, apoiando o desenvolvimento de novos fármacos para a DA.



Sítios de interação do receptor estudados (A); gridbox utilizado no estudo de docking molecular (B).

Agradecimentos/Acknowledgments

Os autores agradecem ao CNPq, Capes, FAPDF e UnB.

Molecular dynamics simulations of interfaces between methyl-methacrylate-based polymers brushes and bacterial outer membrane vesicles

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Palavras Chave:*polymer brushes,outer membrane vesicle,antibacterial,antifouling,interfaces*

Highlights

Molecular dynamics reveals the interaction mechanism between bacterial outer membrane vesicles and polymer brushes.

Cationic brushes enhnace the bacterial vesicles adhesion.

Resumo/Abstract

A potential strategy to reduce bacterial infections associated with implantable medical devices is to coat their surfaces with antibacterial and antifouling polymer brushes. These coatings are formed by highly packed polymer chains that are tethered by one of their ends to a surface. Despite the experimental evidences of the potential of these coatings for reducing the bacterial adhesion, there is a lack of information regarding the molecular understanding of their antibacterial and antifouling activities. The present study aims to analyze interfaces between methyl-methacrylate-based polymers brushes and the bacterial outer membrane (OM) using coarse-grained molecular dynamics (MD) simulations. For the polymer brushes, we evaluated a set with different chemical bahaviors: poly(N,N-dimethyllaminoethyl methacrylate) (pDMAEMA), which is a pH-responsive brush, poly(2 (methacryloyloxy)ethyl)-trimethylammonium chloride) (pMETAC), which is a cationic system, poly([2-(methacryloyloxy)ethyl]dimethyl-(3-sulfopropyl)ammonium) (pMEDSAH), which is zwitterionic, and poly(3-sulfopropyl methacrylate potassium) (pSPMA), which is an anionic system. The bacterial OM was modeled as a bacterial outer membrane vesicle (OMV). The MD simulations of the brush-OMV interfaces revealed two interactions mechanisms: for the cationic brushes, the simulations showed a clear insertion of the OMV in their structure, whereas for the zwitterionic and anionic brushes, the simulations indicated a substantial lateral displacements of the OMV along the surface of these coatings. In addition to an decrease of the brush thickness for the cationic species, we observed an increase of the thickness and sphericity of the OMV during the interaction with four brushes. These results shed light on the molecular details related to the repellent and bacterial effects of these molecular coatings that can assist experimentalists in synthesis optimizations and selection of promising coatings for medical devices.

Agradecimentos/Acknowledgments

This work was supported by Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), Processo n°2023/02556-8.

Monte-Carlo study on chiral emergence of liquid crystals under thermal fluctuations and external electromagnetic fields.

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Palavras Chave:*Gay-Berne Potential, Monte Carlo Simulation, Emergent Properties, Liquid-Crystal, Chirality,Gay-Berne Potential,Monte Carlo Simulation,Emergent Properties,Liquid-Crystal,Chirality*

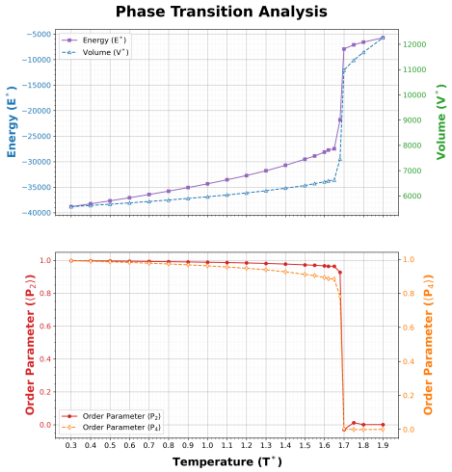
Highlights

The Gay-Berne potential was employed in NpT Monte-Carlo simulations to analyze anisotropic systems. First-order transition was observed at T* ≈ 1.68 from an isotropic fluid to a lamellar crystal.

Resumo/Abstract

The study of anisotropic systems and their response to mirror-symmetry breaking and to external fields provides insight into the physical basis of responsive devices, such as LCD panels and LCoS projectors, which operate through the collective reorientation of their constituent particles along a common direction. The responsiveness of these materials can be attributed, among other factors, to dielectric and magnetic anisotropy. To overcome the computational limitations of atomistic molecular dynamics, these systems can be modeled using the Gay–Berne potential, which allows simulation of discotic and calamitic structures, including nematic, smectic, cholesteric, and chiral-nematic mesophases.

In this work, we investigated the phase behavior of 2048 ellipsoidal particles modeled with Gay–Berne parameters κ = 3.0, κ' = 5.0, μ = 1.0 and ν = 3.0. Monte Carlo simulations at a reduced pressure of p*=0.61 were performed using the DL_MONTE software, employing a linear cooling sweep from T* = 1.90 to T* = 0.30. Analysis of thermodynamic observables and order parameters indicates a first-order phase transition at T* ≈ 1.68, from an isotropic fluid (



Energy (E), Volume (V*) and Order Parameters (,) vs Temperature (T*) at constant pressure.*

Agradecimentos/Acknowledgments

Programa Unificado de Bolsas de Estudos para Apoio à Formação de Estudantes de Graduação (PUB-USP), University of São Paulo. Project Nº 2388.
The authors are also grateful for the HPC resources provided by the Cluster-Department of Chemistry/FFCLRP

New DFT insights into silicalite formation from layered H-magadiite.

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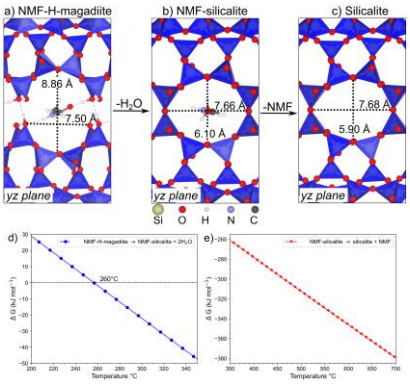
Palavras Chave:*Magadiite,DFT,Silicalite,Thermodynamic*

Highlights

Models for H-magadiite condensation waanalyzed by DFT calculations. The ΔG indicated that the dehydroxylation process starts spontaneously at 260°C. The intermediate 'NMF-silicalite' was observed.

Resumo/Abstract

Na-magadiite is a hydrous layered silicate with a crystalline structure solved through theoretical-experimental characterizations using DFT calculations. However, the acid form, H-magadiite, does not exhibit an adequate stacking orientation of the layers, resulting in its low crystallinity. Therefore, the challenge in obtaining a 3D material from H-magadiite is precisely to maintain the adequate structural configuration of the layers. Thus, this work aims to evaluate the structure of H-magadiite and its condensation steps into a medium-pore solid, here referred to as silicalite, through computational simulations (Figure 1). First, H-magadiite was simulated from Na-magadiite by modifying the interlayer content and preserving the lamella structure. The stacking orientation of the layers was adjusted by geometry optimization, and simulated XRD reproduced an experimental peak near 25º 2θ. In the intercalation of N-methylformamide (NMF) molecules, the optimized NMF-H-magadiite showed a SiOH-O(NMF) distance of 1.44 Å and shorter SiOH-OHSi hydrogen bonds (1.60 Å – 1.73 Å) than H-magadiite (1.65 Å – 1.90 Å). Consequently, the basal spacing changed from 13.02 Å (H-magadiite) to 14.0 Å (NMF-H-magadiite), both in good agreement with the experimental data. In the case of NMF-silicalite and silicalite models, geometry optimizations showed an elliptical pore. Thermodynamic analyses revealed that, during the experimental calcination at 600ºC, dehydroxylation is favorable starting from 260ºC, while the exit of NMF begins at 409º C (Figure 1d and 1e). Thus, NMF-silicalite can be experimentally obtained under specific conditions, such as thermal treatment until temper-atures between 250 – 450º C. Furthermore, the structural transformations of silicalite into dense silica poly-morphs are not thermodynamically favorable. This work sheds light on the structural and thermodynamic conditions of a 3D material from lamellar precursors, which are experimentally poorly understood.



Agradecimentos/Acknowledgments

This work was supported by Sao Paulo State Research Foundation (FAPESP grant number 2023/09485- 9 and 2021/12058-0), and the National Council for Science and Technology (CNPq, grant number 312981/2020-1).

Photocatalytic performance of ZnO and TiO_2-based systems in tetracycline remediation

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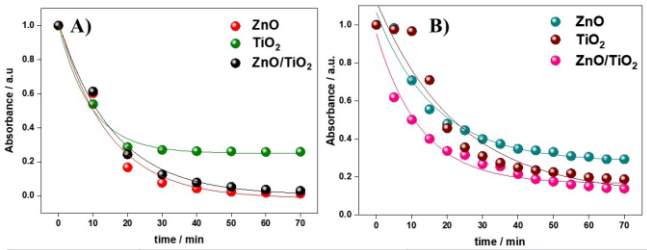
Palavras Chave:*ZnO,TiO2,tetracycline,photocatalysis,emerging contaminants*

Highlights

Obtention of nanomaterials based on ZnO and TiO_2 for tetracycline remediation. Enhanced UV/visible photocatalysis for ZnO/TiO_2. Ecotoxicity and ROS mechanisms were evaluated beyond photocatalysis.

Resumo/Abstract

The increasing occurrence of antibiotics in aquatic environments has raised serious concerns due to their persistence, toxicity, and contribution to antimicrobial resistance. Among these contaminants, tetracycline (TC) is frequently detected in wastewater effluents and is poorly removed by conventional treatment processes. This study investigates ZnO, TiO_2, and ZnO/TiO_2 semiconductor nanomaterials synthesized via a green-chemistry-oriented sol-gel route, aiming at the photocatalytic remediation of TC from aqueous media. The nanomaterials were characterized by UV–Vis, photoluminescence, FTIR, thermal analysis (TGA), X-ray diffraction (XRD), and electron microscopy, confirming the formation of stable semiconductor nanoparticles with wide band gaps and defect-rich structures. Photocatalytic performance was evaluated under UV (365 nm) and visible (465 nm) LED irradiation in a custom-built low-energy photoreactor. ZnO exhibited superior activity under UV light, while ZnO/TiO_2 systems showed enhanced performance under visible irradiation, highlighting the role of heterojunctions in improving charge separation (Fig). Moreover, ZnO/TiO_2 displayed tunable performance depending on the thermal treatment, acting effectively as an adsorbent followed by photocatalyst, or directly as a photocatalyst. Kinetic modeling followed a pseudo-first-order and demonstrated that higher apparent rate constants do not necessarily correspond to higher overall removal. Mechanistic studies revealed that superoxide anion radicals and photogenerated charge carriers play a dominant role in TC degradation, depending on the irradiation regime. Comparative assessments of photocatalysis, photolysis, and TC irradiation alone indicated the formation of persistent aromatic intermediates, evidenced by residual UV absorption. Ecotoxicological assays using*Vibrio fischeri*confirmed that partially degraded solutions may retain environmental toxicity when degradation products exceed concentrations of 12.5 ppm.



C)

Variables	UV 365 nm			Blue light 465 nm		
	ZnO	TiO_2	ZnO/TiO_2	ZnO	TiO_2	ZnO/TiO_2
Removal Efficiency/ %	98.80%	74.27%	96.97%	71.01%	81.46%	86.28%
R^2	0,979	0.994	0.986	0.966	0.922	0.976
k_{ap} /10^{-2} min^{-1}	(8.37±0.408)	N.A*	(7.67±0,551)	(6.049±0.760)	(4.367±1.007)	(7.954±0.766)

N.A* *not applicable (data did not fit the proposed model).*

Kinetics at 374 nm with pseudo-first-order fitting under A) UV, B) blue light; C) fitted parameters

Agradecimentos/Acknowledgments

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Photodegradation of Avobenzone in presence of nonionic surfactants: Impacts on sunscreen formulations

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Palavras Chave:*photodegradation,sunscreens,surfactants,cosmetics.,avobenzone*

Highlights

Physical-chemical studies on Avobenzone photostability. Avobenzone in the presence of nonionic surfactants for application in sunscreens.

Resumo/Abstract

Avobenzone (AVO) is one of the most used UVA radiation filters in sunscreens, absorbing in the ranges of 320 to 400 nm. The protection offered by AVO occurs in its enolic form, however, like most organic filters, the exposure to solar radiation leads to the conversion of the enolic form to the keto form, generating photoallergic and cytotoxic photodegradation products, affecting its effectiveness and impacting the user's health[1],[2]. The usage of nonionic surfactants in this research is based on their low irritability and weak interaction with skin proteins, as well as being low cost and biodegradable, being widely used in cosmetic formulations as an emulsifier and antibacterial agent. The photostability of AVO in the presence of nonionic surfactants was evaluated, with Tween 80, Pluronic® P-123, PEG-35, and PEG-40 (1% w/v) surfactants being chosen for the photodegradation tests. The absorption spectra of UV-Vis spectra were registered after specific periods of time, and the degradation kinetics were adjusted to first-order models. It was observed that AVO presented greater stability and lower photodegradation rate (k) in the presence of PEG-40 and in the presence of P-123, highlighting them as a potential additive in sunscreen formulations due to its better performance. To evaluate the preferential photostability, the binding constant of AVO with the different surfactants (Kb) was evaluated through the absorption intensity of AVO at different concentrations of the surfactants. The binding order was P-123>PEG-35>PEG-40>Tween 80, which is in agreement with the observed stability order. The cmc of surfactants was determined by fluorescence spectroscopy, where the results obtained were close to those found in the literature, demonstrating that the experiment was successful and can be applied in the next stages of the project.

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[2]*Pharmaceuticals*, 2022,**15(3)**, 263

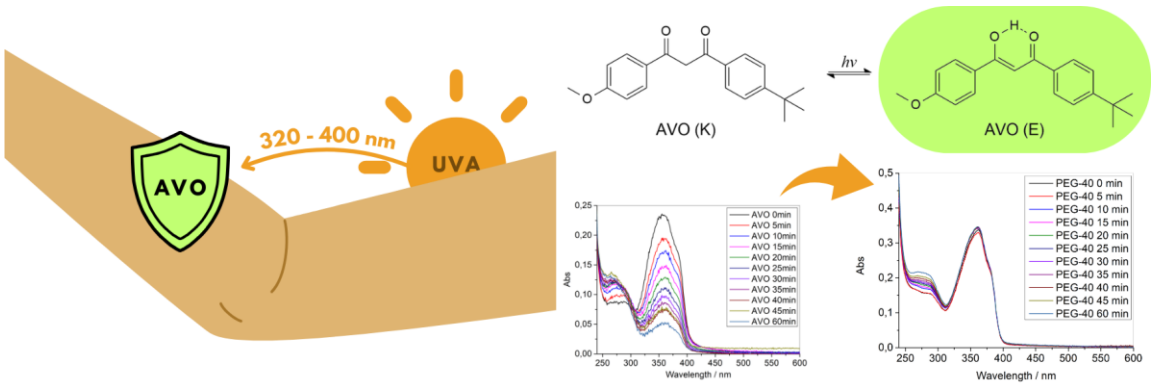


Illustration of Avobenzone as UVA filter and it's UV-Vis spectrum before and after a PEG-40 solution

Agradecimentos/Acknowledgments

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Physicochemical Interpretation of CO2 Adsorption Mechanisms in N-Doped Carbons via Multilayer Perceptron Neural Network

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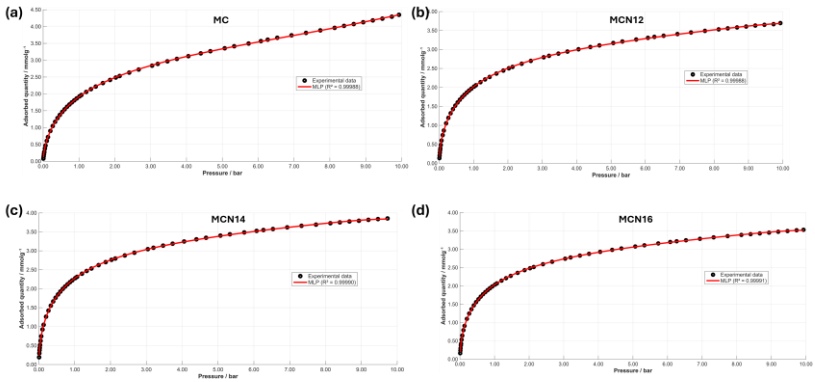
Palavras Chave:*CO2 capture,N-doped mesoporous carbon,Multilayer Perceptron,Adsorption isotherms,Toth model*

Highlights

Sustainable N-doped carbon synthesis; MLP neural network predicts CO2 adsorption with R2> 0.999; MCN14 optimized for 2.3 mmol/g capture capacity; Surface energy heterogeneity validate

Resumo/Abstract

The escalating atmospheric CO_2 concentration remains a primary driver of global climate change, necessitating the development of advanced capture technologies. Adsorption using porous materials offers a cost-effective solution, but enhancing selectivity and modeling accuracy in complex matrices is essential. This study evaluates nitrogen-doped mesoporous carbons (MCNs) synthesized via a sustainable, solvent-free mechanochemical route. This green synthesis approach eliminates the need for toxic solvents, utilizing manual grinding in a mortar and pestle to integrate nitrogen precursors into the carbon matrix To interpret the complex adsorption phenomena and overcome the limitations of classical phenomenological models, a Multilayer Perceptron (MLP) neural network was implemented. The MLP used a personalized architecture activated by physical adsorption models, designed to correlate structural properties with capture performance. By systematically modulating the precursor ratios, the MCN14 material was optimized, exhibiting a nitrogen content of 9.05% and a balanced mesoporous structure. Characterization via SEM/TEM and XPS confirmed the successful doping and high surface area. The MLP network successfully predicted the adsorption isotherms with superior accuracy (R^2 > 0.999), precisely identifying the transition between active nitrogen site saturation and mesopore filling. Results demonstrated that MCN14 reaches a capture capacity of 2.3 mmol·g^{-1} at 1 bar and 298 K, significantly outperforming undoped counterparts. The Toth model confirmed an energetically heterogeneous surface favorable for physisorption with strong interaction sites (t = 0.81). Furthermore, the materials showed a cyclic stability of 99.12%, reinforcing their technical viability. This work validates Artificial Neural Networks as robust tools for the design and optimization of sustainable adsorbents, reducing computational time and experimental costs in carbon mitigation research.



Experimental CO2 adsorption isotherms and MLP neural network predictive curves for MCNs materials

Agradecimentos/Acknowledgments

The authors thank CNPq, CAPES, FAPEMIG, the Chemistry Department/Microscopy Center at UFMG for financial and technical support.

Predicting Rh-103 NMR chemical shift in rhodium complexes with the new NMR-DKH basis set

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Palavras Chave:*Rh complexes, DFT, Computational protocol.*

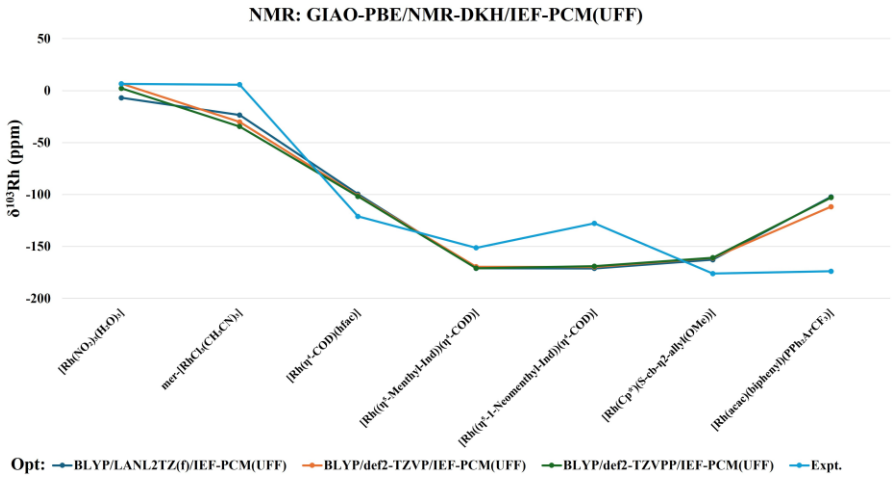
Highlights

A new NMR-DKH basis set for Rh atom was proposed. Calculated δ^{103}Rh with the NMR-DKH basis set showed a good agreement with the experimental values.

Resumo/Abstract

Recently, rhodium (Rh) complexes have been studied due to their anticancer potential. Aiming at the search for new Rh complexes, Nuclear Magnetic Resonance (NMR) spectroscopy is a fundamental tool for the characterization of these complexes and studies of reaction mechanisms and kinetics. Computational prediction of the Rh-103 NMR chemical shift (δ^{103}Rh) is a difficult task, with few studies in the literature. Thus, the present work aims to propose a computational protocol for predicting δ^{103}Rh with the new NMR-DKH basis set. Initially, the NMR-DKH basis set was developed for the Rh atom 1 . After, a set of 50 Rh(III) complexes, presenting experimental δ^{103}Rh ranging from -1,897 ppm to 4,532 ppm, were selected. The structures of the complexes were optimized at the BLYP/RhBS/def2-SVP/IEF-PCM(UFF) level, where RhBS corresponds to the Rh basis sets (LANL2TZ(f), def2-TZVP and def2-TZVPP). Subsequently, δ^{103}Rh was calculated using the equation δ ^{03}Rh = a x σ^{103}Rh + b, where the coefficients a and b were obtained from the linear regression model between the nuclear shielding constant of Rh-103 (σ^{103}Rh) calculated at the GIAO-PBE/NMR- DKH/IEF-PCM(UFF) level and the experimental δ^{103}Rh. Considering the calculated data for seven Rh(III) complexes, coefficients of determination (R^2) of 0.76, 0.79, and 0.75 were obtained with the structures optimized with RhBS = LANL2TZ(f), def2- TZVP, and def2-TZVPP, respectively. The comparison between the calculated and experimental δ^{103}Rh values (Figure 1) shows that the calculated values adequately describe the behavior of the experimental values, indicating a good fit of the proposed odels. In the next steps, NMR data from the remaining Rh(III) complexes will be included, as well as an evaluation of the role of the DFT functional.

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Calculated δ103Rh for a set of seven Rh(III) complexes

Agradecimentos/Acknowledgments

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Predicting 13C NMR chemical shift in Bi(III) complexes: a theoretical and experimental study

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Palavras Chave:*Bismuth complexes,DFT,Basis sets,NMR-DKH*

Highlights

A new NMR-DKH basis set was proposed for Bi atom.

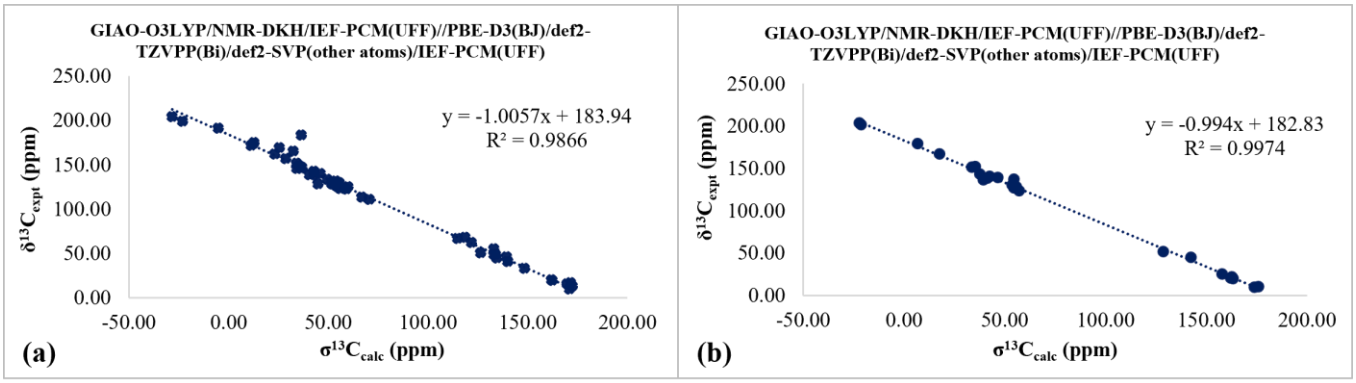
Computational protocols for predicting the δ¹³C in Bi(III) complexes were proposed and validated.

Resumo/Abstract

Bismuth(III) complexes have attracted growing interest due to their applications in coordination chemistry and materials science. However, computational prediction of ¹³C NMR chemical shifts (δ¹³C) remains challenging for Bi(III) systems. Herein, we report the development of a new all-electron basis set for bismuth, denoted NMR-DKH, and a robust computational protocol for predicting the δ¹³C in Bi(III) complexes. The influence of exchange-correlation functionals was systematically evaluated for geometry optimization and NMR calculations using a training set of Bi(III) complexes (59 ¹³C signals), with model performance assessed using established structural and NMR accuracy descriptors. Geometry optimizations were best described at the PBE-D3(BJ)/def2-TZVPP(BiBS)/def2-SVP(LBS)/IEF-PCM(UFF) level, while δ¹³C values showed optimal agreement with experiment using the GIAO-O3LYP/NMR-DKH/IEF-PCM(UFF) approach. For this NMR//Geometry protocol, the training set yielded a mean absolute deviation (MAD) of 3.70 ppm, a standard deviation of the absolute deviations (SDAD) of 4.99 ppm, and a coefficient of determination (R^2) of 0.9866. High predictive accuracy was retained upon external validation with an independent set of Bi(III) complexes (24 ¹³C signals), affording MAD = 2.32 ppm, SDAD = 0.91 ppm, and R^2 = 0.9974. Subsequently, a newly Bi(III) complex was experimentally synthesized and characterized. The proposed computational protocol for δ¹³C was applied in studying this complex, resulting in δ¹³C values with absolute deviations of 0.44-3.59 ppm (MAD = 2.33 ppm, SDAD = 0.91 ppm, R^2 = 0.9882), supporting its structural assignment. Overall, this work establishes an efficient method for calculating δ¹³C in Bi(III) complexes based on the GIAO-O3LYP/NMR-DKH/IEF-PCM(UFF)//PBE-D3(BJ)/def2-TZVPP(BiBS)/def2-SVP(LBS)/IEF-PCM(UFF) protocol.

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Calculated σ13C vs. experimental δ13C for (a) training and (b) validation sets of Bi(III) complexes

Agradecimentos/Acknowledgments

FAPERJ (E-26/201.336/2022 – BOLSA JCNE and E-26/210.070/2022 – DCTR) CNPq (Financial code 140579/2025-7), and CAPES (Finance Code 001).

Predicting the Copper-63 NMR chemical shift in Cu(I) complexes using the new NMR-ZORA basis set

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Palavras Chave:*Nuclear Magnetic Resonance,Cu-63 Nucleus,DFT,basis set,Relativistic Effects*

Highlights

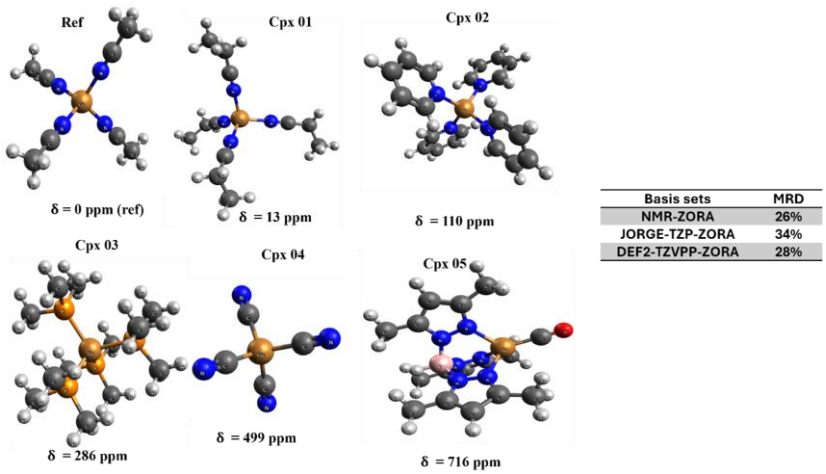
The new TZ2P Gaussian basis set named as NMR-ZORA for the copper atom was proposed and evaluated.

The protocol GIAO-PBE0-SC-ZORA/NMR-ZORA/CPCM//M11-SC-ZORA/NMR-ZORA/CPCM showed the best results.

Resumo/Abstract

Nowadays, copper complexes are widely studied in the pharmaceutical industry for their potential anticancer activity[1] . In nuclear magnetic resonance (NMR) spectroscopy, although the copper-63 nucleus has high natural abundance, which makes it more detectable compared to other nuclei, the tetrahedral geometry of Cu(I) complexes makes the calculations extremely sensitive to the chemical environment. In this way, advances in computational chemistry make it possible to analyze and evaluate new compounds more effectively[2]. In the present study, computational protocols for predicting the Cu-63 NMR chemical shift (δ 63 Cu) in Cu(I) complexes were proposed using the new NMR-ZORA basis set[3] . The geometries were optimized at DFT-Functional-SC-ZORA/NMR-ZORA/CPCM level, considering a set of 21 functionals. The δ 63 Cu were calculated at GIAO-PBE0-SC-ZORA/NMR-ZORA/CPCM level. The jorge-TZP-ZORA and ZORA-def2-TZVP basis sets were also considered for both geometry and NMR. The [Cu(NCMe) 4] +1 complex, in MeCN, was used as reference in calculating the δ 63 Cu. All calculations were carried out in ORCA 6.1.0 program. The calculated results showed that the δ 63 Cu is very sensitive to the DFT functional employed in both optimization and NMR calculations. The proposed model with the lowest mean relative deviation (MRD = 26%) was GIAO-SC-ZORA-PBE0/NMR-ZORA/CPCM//SC-ZORA-M11/NMR-ZORA/CPCM. Furthermore, the results obtained demonstrate the role of the NMR-ZORA basis sets, which provided a better description of δ 63 Cu than other basis sets in the literature, with the same DFT functional. In the next steps, a larger number of complexes will be evaluated, as well as an analysis of the DFT functional in the NMR calculations.

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Basis sets	MRD
NMR-ZORA	26%
JORGE-TZP-ZORA	34%
DEF2-TZVPP-ZORA	28%

Copper (I) complexes studied in the present work.

Agradecimentos/Acknowledgments

FAPERJ ((E-26/201.336/2022 – BOLSA JCNE), CNPq, and CAPES (Finance Code 001).

Predicting the first hyperpolarizability of amino-substituted chromophores using the new nqtcm-VDZP basis sets

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Palavras Chave:*Non-Linear Optics,,Photonic,DFT,Chromophores*

Highlights

The geometries of a set of 15 molecules were optimized with 30 different DFT functionals. The first hyperpolarizability was evaluated with the new nqtcm-VDZP basis sets

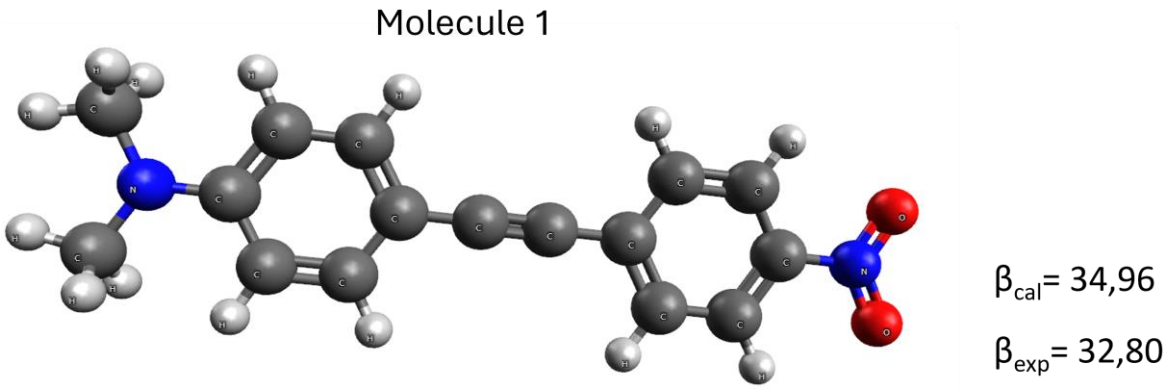
Resumo/Abstract

Nonlinear optics (NLO) plays a central role in the development of materials for photonics and optoelectronic applications, with first molecular hyperpolarizability (β) being one of the fundamental properties[1]. However, reliable theoretical prediction remains challenging due to its high sensitivity to the choice of DFT functional, basis sets, and solvent effects. In this work, we computationally investigate the quality of nqtcm-VDZP basis sets in predicting the first hyperpolarizability of a series of chromophores containing dialkylamine and diarylamine donor amino groups. Initially, the nqtcm-VDZP basis sets for H-He, Li-Ne, and Na-Ar were proposed[2]. After, a set of 15 molecules containing amino donor groups and presenting β values ranging from 32.8 x 10^{-30} esu to 119 x 10^{-30} esu were selected[3]. The structures were optimized at the DFT-Functional/def2-SVP/IEF-PCM(UFF) level, considering a set of 30 DFT functionals. Subsequently, the β values were calculated at CAM-B3LYP/nqtcm-VDZP/IEF-PCM(UFF) level. All calculations were performed using the GAUSSIAN 16 Rev. C. 01 program. The calculated structures do not show significant variations regarding the used DFT functional. However, the β values proved to be very sensitive to changes in geometry. For molecule 01, the calculated values show relative deviations from the experimental values ranging from 6.58% (Opt LC-BLYP) to 51.00% (Opt BLYP). Overall, the largest deviations in β values were observed when GGA functionals were used in the structural description, with long-range corrected functionals resulting in the smallest deviations. In the next steps, the first hyperpolarizability will be calculated for the other molecules and correlated with structural and electronic parameters, aiming to observe the role of molecular structure in modulating β values.

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[2]Paschoal, D. et al., Int J Quantum Chem 2014, 114, 796-804.

[3]Moylan, C., J Am Chem Soc 1993, 115, 12599-12600.



Experimental and calculated beta (β) values at CAM-B3LYP/nqtcm-VDZP//LC-BLYP/def2-SVP level

Agradecimentos/Acknowledgments

FAPERJ ((E-26/201.336/2022 – BOLSA JCNE), CNPq, and CAPES (Finance Code 001).

Preparo e caracterização físico-química de sistemas coloidais presentes na biomassa oriunda da produção de etanol de milho

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Palavras Chave:*Óleo de milho, Emulsões de Pickering, Sistemas coloidais, Recuperação de óleo e Estabilidade interfacial.*

Highlights

Stabilization in corn emulsions, multitechnique characterization of particles and interfaces, basis for efficient corn oil recovery strategies.

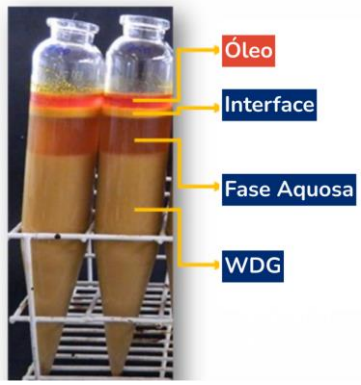
Resumo/Abstract

O*Wet Distillers Grains*(WDG) é um coproduto úmido da produção de etanol a partir do milho, composto por água, óleo residual, proteínas e material particulado de origem vegetal, configurando um sistema coloidal complexo. Embora apresente elevada estabilidade, que dificulta a recuperação do óleo mesmo na presença de desestabilizantes industriais, os mecanismos físico-químicos responsáveis por essa estabilidade ainda são pouco compreendidos. A recuperação do óleo de milho presente no WDG é de interesse econômico e estratégico, contribuindo para a valorização do coproduto e para a sustentabilidade da cadeia produtiva do etanol. Dessa forma, torna-se essencial compreender os mecanismos que dificultam a desestabilização dessa emulsão.

Este trabalho investiga a hipótese de que partículas sólidas suspensas no WDG atuem como agentes estabilizantes de emulsões óleo/água por um mecanismo análogo ao das emulsões de Pickering, no qual partículas se adsorvem à interface e reduzem a coalescência das gotas. Considera-se também a contribuição de outros componentes com atividade interfacial, incluindo compostos orgânicos presentes no próprio óleo de milho, que podem atuar de forma isolada ou sinérgica com as partículas sólidas.

Para simular o WDG, foram preparadas emulsões-modelo com diferentes proporções de óleo e partículas. A metodologia experimental inclui microscopia óptica, difração a laser, avaliação de estabilidade ao longo do tempo e por métodos acelerados, reologia, potencial zeta, ressonância magnética nuclear e espectroscopia de infravermelho por transformada de Fourier.

A partir dos resultados obtidos, serão elucidados os mecanismos responsáveis pela estabilização das emulsões presentes no WDG, fornecendo a base científica para a proposição de estratégias de desestabilização controlada, com vistas à separação eficiente e à recuperação do óleo de milho. Esses avanços contribuem para a valorização do coproduto e para a sustentabilidade da cadeia produtiva do etanol.



Separação parcial de fases no WDG, evidenciando fase oleosa, interface e fase aquosa.

Agradecimentos/Acknowledgments

Os autores agradecem o apoio da CNPq, da PUC-Rio, da Indorama Ventures e à organização da SBQ pela oportunidade de apresentar este trabalho.

Probing the membrane diffusion of quinolinic drugs: a steered molecular dynamics study

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Palavras Chave:*Free Energy Profile, Umbrella Sampling, Membrane permeation, DMPC bilayer,Free Energy Profile,Umbrella Sampling,Membrane permeation,DMPC bilayer*

Highlights

Steered MD and umbrella sampling map the free-energy landscape of CQ, AQ and PQ permeation through a DMPC bilayer in multiple protonation states.

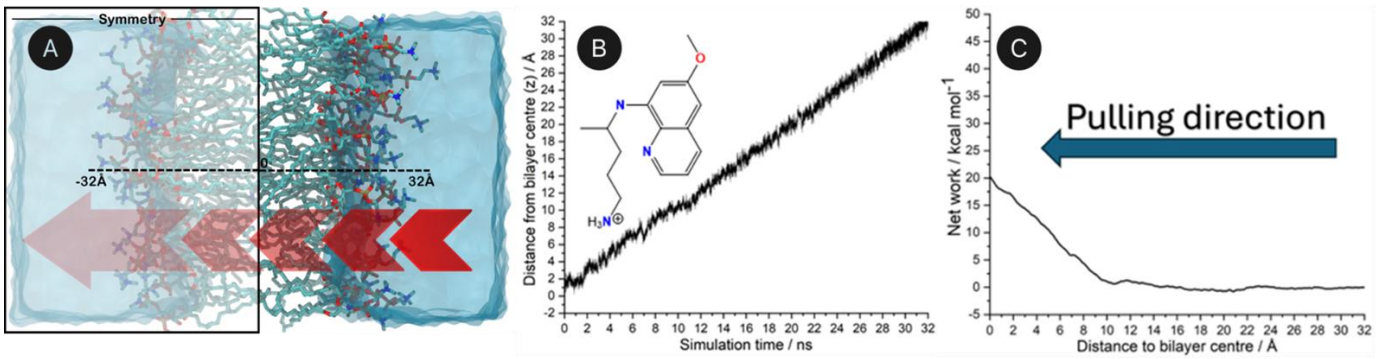
Resumo/Abstract

Malaria remains a critical global health burden, exacerbated by the emergence of*Plasmodium*strains resistant to classic therapies. Quinoline-based agents, such as chloroquine (CQ), amodiaquine (AQ), and primaquine (PQ), have long served as frontline defences. These compounds function primarily by accumulating in the parasite's food vacuole, inhibiting the detoxification of free heme into hemozoin[1]. Physiologically, these drugs behave as weak bases, existing in a pH-dependent equilibrium between neutral, mono-, and diprotonated forms. Conventionally, drug uptake is described by the "ion-trapping" model: the lipophilic neutral form enters the erythrocyte via passive diffusion, becomes protonated in the acidic vacuole (pH ~4.5), and is trapped due to the membrane's perceived impermeability to charged species[2–3]. In this work, we employed Molecular Dynamics (MD) simulations supported by Umbrella Sampling to investigate the permeation profiles of CQ, AQ, and PQ across a membrane bilayer (Fig. 1). We are working on the evaluation of free energy profiles for pH 7 and neutral protonation states. Even though results are still being obtained and analysed, we have so far simulated all compounds though the membrane and we are currently sampling the space for the umbrella sampling procedure. SMD pulling yields accumulated work to the bilayer centre of 22.23 kcal mol−¹ (CQ), 25.85 kcal mol−¹ (AQ) and 14.20 kcal mol−¹ (PQ) for the neutral species. For protonated forms, PQH^+ shows lower accumulated work (20.13 kcal mol−¹) than AQH^+ (38.95 kcal mol−¹) and CQH_2^{2+} (41.70 kcal mol−¹). Based on our preliminary findings, neutral quinolines tend to adopt configurations in which the aromatic scaffold is stabilized in the apolar region and protonated forms interact strongly with lipid headgroups.

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(2) Ginsburg, H.;*at al.*,*Biochem. Pharmacol.***1991**,*41*(10), 1463–1470

(3) Hayward, R.;*at al.*,*J. of Cell Sci.***2006**,*119*(6), 1016–1025



SMD/umbrella sampling setup for PQ permeation in DMPC (PMF z: ±32 Å)

Agradecimentos/Acknowledgments

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Rational Design of MIPs for the analytes TBBPA and DBP via DFT and Surface-Mapping Conformational Screening

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Palavras Chave:*DFT,MIPs,Microplastic,Tetrabromobisphenol A,Dibutyl Phthalate*

Highlights

Rational design via DFT optimized MIPs for hazardous plastic additives, cutting down experimental costs and material waste.

Resumo/Abstract

With global population growth, plastic consumption has increased rapidly, and inadequate collection and disposal have intensified environmental accumulation [1]. Over time, these persistent materials fragment into microplastics (MPs), which are difficult to detect and quantify in complex environmental matrices [1–3]. Molecularly Imprinted Polymers (MIPs) provide a stable, low-cost recognition layer for sensors designed to monitor these contaminants [4]. In imprinting, pre-polymerization analyte–functional monomer complexes (mainly noncovalent) guide selective cavity formation after polymerization and template removal, while the structural monomer mainly ensures morphology [5,6]. To rationalize synthesis and reduce empirical trial-and-error, this study employed Density Functional Theory (DFT) to evaluate the stability of pre-polymerization complexes for MIPs targeting TBBPA (*tetrabromobisphenol A*) and DBP (*dibutyl phthalate*). All geometries were optimized in gas phase using ORCA at the B3PW/def2-SVP level, and monomer–analyte conformations were generated using the Molecular Binding Algorithm by Surface Mapping (MBASM). Frequency calculations on isolated molecules confirmed true minima. The simulations indicated that, for TBBPA, 4-imidazole acrylic acid (4imid) showed the most favorable interaction energy (−0.87 eV), supporting the selection of a semi-covalent imprinting route. For DBP, 4-vinylpyridine (4VP) yielded the best performance (−0.67 eV) and was selected for the noncovalent route. Divinylbenzene (DVB) was chosen as the structural monomer for both systems, with interaction energies of −0.73 eV (TBBPA) and −0.72 eV (DBP), ensuring matrix stability while minimizing competition with analyte–functional monomer interactions; in addition, the relative concentrations of each component are critical for achieving selective recognition. Overall, this computational strategy enables the rational selection of MIP components toward highly selective electrochemical sensors.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP (Grant No. #2024/12623-7) and the Institute of Chemistry (IQ–USP), University of São Paulo.

Síntese e caracterização físico-química de bioplásticos à base de celulose extraída de Cola acuminata utilizando diferentes agentes poliméricos

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Palavras Chave:*Biomassa lignocelulósica; Físico-química; Caracterização, py-GC-MS,: Biomassa lignocelulósica,Físico-química,Caracterização,py-GC-MS,FT-IR*

Highlights

Potential of*Cola acuminata*as an alternative and renewable source for bioplastics.

Resumo/Abstract

Bioplásticos biodegradáveis foram sintetizados a partir de celulose extraída da casca de*Cola acuminata*(OBI), utilizando diferentes agentes poliméricos: carboximetilcelulose (CCMC), goma-laca (CGL) e goma xantana (CGX). A celulose foi obtida por tratamento alcalino e empregada como matriz polimérica. Os bioplásticos foram preparados pelo método de*solvent casting*, com adição de glicerol como plastificante e secagem controlada. Todas as formulações resultaram em filmes contínuos e estruturalmente estáveis.

O bioplástico CCMC apresentou maior homogeneidade e flexibilidade, atribuídas à afinidade química entre os grupos hidroxila da celulose e os grupos carboximetila da CMC. O sistema CGL exibiu maior rigidez e menor afinidade com água, em função da presença de grupos éster e constituintes hidrofóbicos da goma-laca. O bioplástico CGX demonstrou boa integridade estrutural, associada à elevada capacidade de formação de rede da goma xantana.

A caracterização por espectroscopia no infravermelho com transformada de Fourier (FTIR) evidenciou interações intermoleculares em todas as amostras, com alargamento da banda O–H (3200–3400 cm^{-1}) e presença de bandas C–O–C e C–O (1000–1150 cm^{-1}). Bandas de carboxilato (~1600 cm^{-1}) foram observadas nos bioplásticos CCMC, enquanto bandas de carbonila (1700–1730 cm^{-1}) confirmaram a incorporação da goma-laca nos sistemas CGL. A difração de raios X (DRX) indicou padrão típico de celulose tipo I, com redução do índice de cristalinidade após a formação dos bioplásticos, mais pronunciada nos sistemas CCMC e CGX.

A análise por Py-GC-MS revelou perfis distintos de degradação térmica, confirmando a incorporação dos diferentes agentes poliméricos. Os bioplásticos obtidos apresentam potencial para aplicações em embalagens biodegradáveis, revestimentos naturais e materiais agrícolas, além de contribuir para a valorização de um resíduo lignocelulósico vegetal e a substituição de matérias-primas fósseis.

Agradecimentos/Acknowledgments

Ao Programa de pós-graduação em química Aplicada da Universidade do Estado da Bahia (UNEB) pela infraestrutura disponível, CAPES pela bolsa de pós-doutorado

Simple Colorimetric Detection Method for Carbendazim via Derivatization

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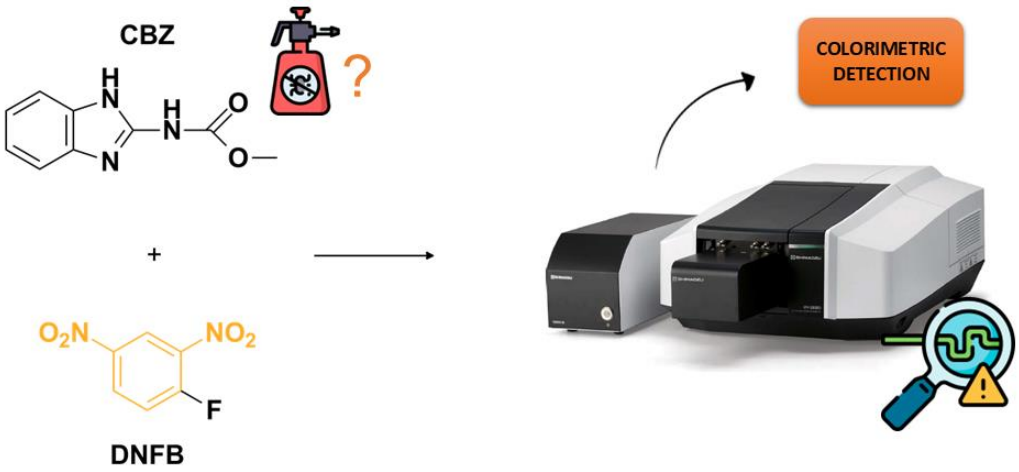
Palavras Chave:*Pesticide,kinectic studies,benzimidazoles,1-fluoro-2,4-dinitrobenzene,UV-Vis spectrometry*

Highlights

• Promoting environmental security through colorimetric detection of carbendazim based on derivatization.
• Kinetic studies on the reaction based on UV-Vis spectrometry data.

Resumo/Abstract

Carbendazim (CBZ) is a widely used systemic fungicide whose use has been banned in Brazil due to concerns related to its toxicity, being classified as mutagenic and carcinogenic. The most commonly employed analytical methods for carbendazim detection are costly, while low-cost alternatives still present limitations in terms of sensitivity and applicability. In this context, the aim of this study is to develop a simple, low-cost, and highly accurate method for carbendazim detection. A colorimetric detection approach is proposed based on the derivatization of CBZ with 2,4-dinitrofluorobenzene (DNFB). Detection was performed using UV-Vis spectrometry, and the obtained data were used for kinetic studies under pseudo-first-order conditions. From the time-resolved spectra, the formation of a characteristic absorption band with a maximum in the 325-370 nm range was observed. Initial assays using pure carbendazim samples indicated that the reaction is favored under neutral to slightly basic conditions, with pH 7.5 identified as the optimal condition. Subsequently, the method was applied to commercial formulations, showing improved performance in the pH range between 7.5 and 9. Within this pH range, no hydrolysis products of the studied species were observed, demonstrating the selectivity of the method toward DNFB. Additional studies are currently underway to optimize the reaction conditions and further improve the method performance. The results obtained so far indicate that the proposed methodology has strong potential as a simple, efficient, and low-cost approach for carbendazim detection.



Schematic representation of the colorimetric detection of CBZ using DNFB as a derivatizing agent.

Agradecimentos/Acknowledgments

UFPR, CAPES, Finep, CNPq, PhosAgro/Unesco/IUPAC, Fundação Araucária, L'Oréal-UNESCO-ABC, INCT NanoVida, INCT Nanocarbono e Materiais 2D.

Structural and functional effects of W/O/W emulsion–encapsulated NADES annatto seed extract on potato starch films

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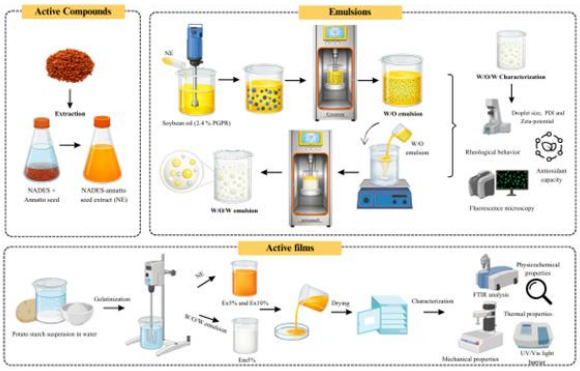
Palavras Chave:*bioactive compounds, encapsulation, active food packaging, radiation barrier, antioxidant activity.,bioactive compounds, encapsulation, active food packaging, radiation barrier, antioxidant activity.,bioactive compounds,encapsulation,active food packaging,radiation barrier,antioxidant activity*

Highlights

NADES enabled green extraction of annatto seeds
W/O/W emulsions preserved antioxidant activity.
Emulsions reduced moisture and vapor permeability.
W/O/W structuring enhanced UV–Vis barrier properties.

Resumo/Abstract

Biopolymer-based packaging has emerged as a sustainable alternative to conventional plastics; however, high moisture sensitivity and limited barrier performance still restrict its practical application. This study proposes an active packaging strategy integrating green extraction and structured encapsulation technologies to improve the stability and functionality of starch-based films. Annatto (Bixa orellana L.) seed extract was obtained using natural deep eutectic solvents (NADES) composed of choline chloride and lactic acid, representing an environmentally friendly extraction approach. The extract was encapsulated in water-in-oil-in-water (W/O/W) double emulsions and incorporated into potato starch-based films. The physicochemical, colorimetric, rheological, and antioxidant properties of W/O and W/O/W emulsions were evaluated. The W/O/W system exhibited larger droplet size, pronounced pseudoplastic behavior, and higher physical stability while preserving antioxidant activity, indicating effective protection of the bioactive compounds. When incorporated into starch films, the W/O/W emulsions reduced moisture content and water vapor permeability, suggesting improved resistance to water diffusion. In addition, films containing encapsulated extract showed enhanced UV–Vis light shielding and higher antioxidant efficiency compared to films formulated with non-encapsulated extract. Microstructural, X-ray diffraction, and thermal analyses demonstrated that the presence of W/O/W emulsions modified matrix morphology and crystallinity without compromising film integrity. Overall, W/O/W emulsions act not only as delivery systems but also as microstructural design elements capable of improving transport properties and functional performance. The combination of NADES-based extraction and double emulsion encapsulation represents a promising strategy for developing efficient and sustainable starch-based active packaging materials.



Schematic representation of starch-based active film production.

Agradecimentos/Acknowledgments

The authors acknowledge FAPESP for grants (2020/08727-0; 2024/02072-3) and scholarships to S.K.B., F.P.S., and L.T.; CNPq for a research fellowship to B.C.M. and postdoctoral support to L.T.; and CAPES (Finance Code 001) for partial funding.

Structure-Driven Pathway Shift in Reactions of Organophosphate with Methyl- Imidazoles

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Palavras Chave:*Catalysis, organophosphates, pesticide, nucleophile, degradation*

Highlights

Organophosphates react via attack on the P and/or C atom, depending on the identity of P=X

The position of the methyl group controls the reactivity and regioselectivity for these reactions.

Resumo/Abstract

Organophosphorus pesticides are highly toxic, and their nucleophilic degradation pathways are extremely sensitive to subtle structural changes, such as P=O/P=S identity and nucleophile substitution, which can redirect reactivity from phosphorus to carbon centers and alter both mechanism and product distribution. Imidazole derivatives (x-MEI) can act as N-nucleophiles whose electronic modulation influences both the reaction rate and regioselectivity, highlighting the importance of a correct understanding of these mechanisms for efficient degradation. In this work, we evaluate the mechanistic changes in OPs with P=O and P=S groups in the presence of imidazole and methylated derivatives (1-methylimidazole (1-MEI), 2-methylimidazole (2-MEI), and 4(5)-methylimidazole (4(5)-MEI)), as we observed that non-saint groups also influence the reactivity of these molecules. Kinetic analyses and product characterization are being employed, and the results obtained reveal substrate-dependent mechanistic changes and show that both the nature of the P=X bond and the imidazole substitution pattern control regioselectivity, contributing to the understanding of structure-reactivity relationships in these systems. The results obtained reveal substrate-dependent mechanistic changes and show that both the nature of the P=X linkage and the imidazole substitution pattern control regioselectivity. For all x-MEIs, the attack pathway on the aliphatic carbon proved to be the main reaction route, with the formation of DMPT and leading to the methylation of x-MEIs under mild reaction conditions. Only 2-MEIs and 4(5)-MEIs exhibit phosphorus attack, with the formation of p-nitrophenol (PNP). Studies involving Op with P=O linkage are ongoing. These observed differences highlight the importance of understanding the mechanistic reactions of organophosphates to ensure effective detoxification and reliable and safe monitoring.

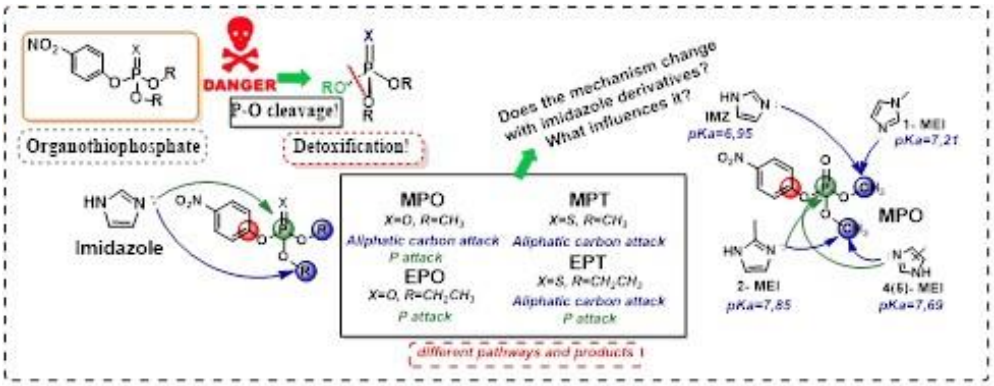


Figure 1 – Overall summary of the studies carried out herein

Agradecimentos/Acknowledgments

UFPR, CAPES, CNPq, L'Oréal UNESCO-ABC, PhosAgro/UNESCO/IUPAC, INCT NanoVida, INCT Nanocarbono e Materiais 2D

Synthesis, Structural Characterization and Luminescent Activity of 2-D Nd(III), Eu(III) and Er(III) Coordination Polymers

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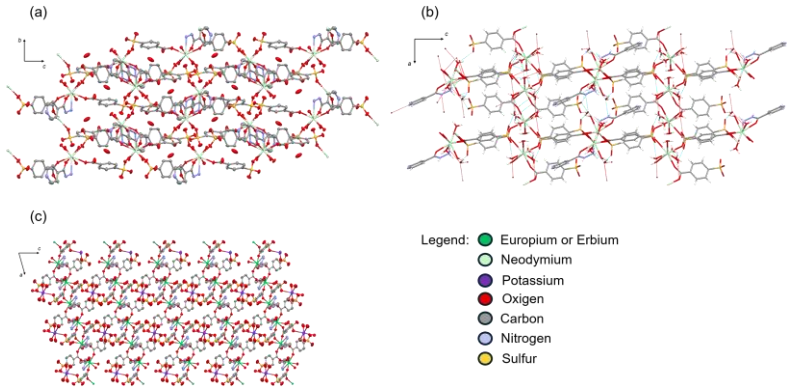
Palavras Chave:*Coordination Polymers,Rare Earths,Isoniazid,4-Sulfobenzoate,X-ray Diffraction by Single Crystal*

Highlights

Structure-property relationships in 2D Nd(III), Eu(III) and Er(III) coordination polymers reveal how distinct crystal structures, built from the same ligands, give different luminescence responses.

Resumo/Abstract

Rare-earth coordination polymers (RE-CPs) are attractive materials for luminescent applications due to the antenna effect promoted by the use of lanthanide ions associated with ligands featuring high π-conjugation, such as carboxylic, aromatic or nitrogenous compounds, like the divergent ligands 4-sulfobenzoate (PSB) and pyridine-4-carbohydrazide – known commercially as isoniazid – (INH). These ligands have already been reported in the literature exhibiting luminescent capability when incorporated into coordination networks. Furthermore, due to the structural variability promoted by the high coordination number of rare earth metals and the coordination possibilities of PBS and INH ligands, several different coordination networks occur, leading to different physicochemical properties. Thus, the structural study of coordination polymers is essential for evaluating the properties exhibited by these materials, enabling the structure-property connection. In this context, this work introduces the synthesis, the characterization and the evaluation of luminescent activity of four novel RE-CPs, built by PBS and INH ligands, and Nd^{3+}, Eu^{3+} and Er^{3+} ions. Two neodymium polymers (Nd-PBS-INH-1 and Nd-PBS-INH-2) with different crystalline structures were obtained, while the europium (Eu-K-PBS-INH) and erbium (Er-K-PBS-INH) polymers are isostructural and feature the presence of a potassium ion, which promotes the two-dimensionality and charge neutralization of the network. Photoluminescent studies reveled that neodymium polymers exhibit characteristic near-infrared emission, with variations in intensity and spectral profile reflecting subtle differences in the coordination environment and crystal field effects. In contrast, the europium and erbium coordination polymers show predominantly ligand-centered emission in the visible region, indicating inefficient energy transfer to the metal center.



Packing of (a) Nd-PBS-INH-1, (b) Nd-PBS-INH-2 and (c) Eu-PBS-INH and Er-PBS-INH polymers.

Agradecimentos/Acknowledgments

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The evolution of reaction pathways of irradiation in H_2O:O_2 ice, driven by temperature

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Palavras Chave:*Reaction pathways,Effective rates (ERCs),Chemical equilibrium,PROCODA code,Astrochemistry*

Highlights

Temperature influences changes in reaction pathways

Radiation dominates the formation of O_2/HO_2, and the destruction of H_2O_2/O_3

ERCs provide constants applicable to astrochemical models and observations

Resumo/Abstract

The evolution of dominant reaction pathways in the formation and destruction of species such as H_2O, O_2, HO_2, H_2O_2, O_3 and HO_3in H_2O:O_2 (6:1) ices irradiated with 0.8 MeV protons at 9 K, 50 K and 100 K was investigated. This was conducted using cosmic rays. The utilization of FTIR-derived column densities from Cooper et al. (2008) (fluence up to 8.2×1014 eV cm^{-2}; ~3 μm thick films) and kinetic modelling employing the PROCODA code is pivotal to the study. The objective of this study was to identify the main pathways at chemical equilibrium (CE) and to track their dose evolution (t = 7–6800 s) via coupled differential equations incorporating reactions of dissociation, bimolecular, and desorption. The validity of this approach is evidenced by its capacity to optimize effective reaction coefficients (ERCs) and its alignment with experimental data.

Temperature is an influential factor on the pathway of production and consumption of species. Hydrogen peroxide (H_2O_2) exhibits a shift from radiolytic (r_{17} at 9 K) to bimolecular (r_{101} at 50 K) and subsequent reversion to radiolytic (r_{35} at 100 K). The formation of O_2 is predominantly facilitated via radiation (r19, r29) across the entire temperature range. The destruction of H_2O_2 transitions from a bimolecular reaction (r172 at 9 K) to radiolysis (r29/r35 ≥50 K).

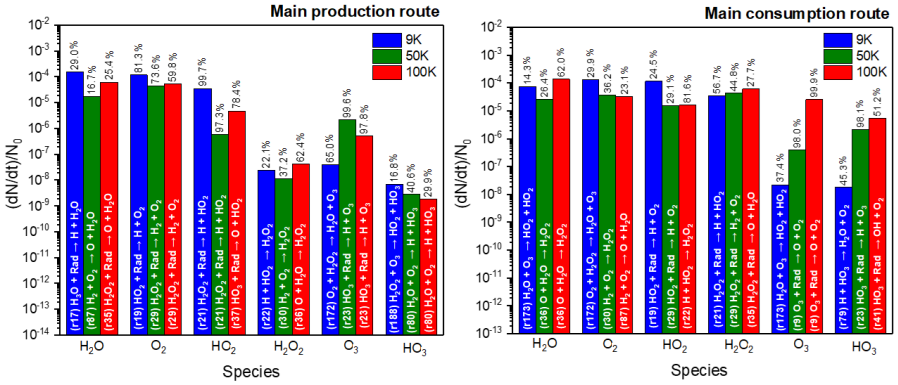
In the lower temperature condition, radiolytic channels predominate, while radical recombination reach their peak at 50K. This phenomenon is of significant importance in the context of the shaping of oxidant yields within astrophysical ices applicable to Europa, the poles of the moon, comets, and dense clouds.

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Silva, J. R. C., Queiroz, L. M. S. V., Ferrão, L. F. A., et al. 2025, ApJ, 985, 254

Silva, J. R. C., Queiroz, L. M. S. V., Ferrão, L. F. A., et al. 2026 (under revision - APJAAS69416 R1)



Main production and consumption reaction rates of the six species at three different temperatures

Agradecimentos/Acknowledgments

The authors acknowledge the CNPq (grants 407124/2022-5, 351261/2023-0, 351650/2023-7, 302939/2022–9, 302608/2022-2, 316874/2023-0), FAPESP (grant 2024/05115-5), and CAPES (grant 88887.919586/2023-00)

Theoretical Evaluation of Monoclinic Ca2Nb2O7

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Palavras Chave:*Calcium niobate,Density Functional Theory (DFT),Monoclinic phase,Electronic structure,QTAIM analysis*

Highlights

Monoclinic $Ca_2Nb_2O_7$ exhibits insulating behavior with a 4.67 eV indirect band gap, where Nb–O bond covalency is governed by local NbO_6 octahedral distortions, as revealed by DFT calculations.

Resumo/Abstract

The monoclinic phase of calcium niobate ($Ca_2Nb_2O_7$), belonging to the$P2_1$space group, has attracted interest for several technological applications [1]. In this work, this phase is investigated through calculations based on Density Functional Theory (DFT), using the CRYSTAL17 program. The atomic description employed the B3LYP-D3 hybrid functional and TZVP basis sets. The protocol included full geometric optimization of the structure, followed by the calculation of vibrational frequencies and the simulation of the Raman spectrum. The electronic structure was characterized by band structure and projected density of states (PDOS), while the nature of the Nb-O and Ca-O bonds was explored through QTAIM topological analysis using the TopIso3D program. The optimized structural parameters showed good agreement with experimental data. The simulated Raman spectrum provided the spectroscopic fingerprint of the phase, with a prominent mode around 800 cm^{-1}. From an electronic standpoint, the material exhibited insulating behavior, with an indirect band gap of 4.67 eV, with the valence band dominated by oxygen orbitals and the conduction band predominantly composed of niobium orbitals. The QTAIM analysis revealed variations in the covalent character of the Nb-O bonds. Such fluctuations were correlated with local distortions in the NbO_6 octahedra, where different interatomic distances modulate orbital overlap and, consequently, the degree of electron sharing in the crystalline lattice.

[1] YANG, Jun et al. Electronic structure, anisotropic elastic and thermal properties of monoclinic Ca2Nb2O7. Ceramics International, v. 42, n. 8, p. 9426-9432, 2016.

Agradecimentos/Acknowledgments

CNPQ and PROPESQ-UFPB

Theoretical investigation of the mechanisms of multicomponent reactions catalyzed by β-cyclodextrin in aqueous solution

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Palavras Chave:*Supramolecular catalysis, pyrido[2,3-d]pyridines, QM:QM method; reaction mechanism*

Highlights

This work presents a complete theoretical elucidation of the mechanism reaction of formation of pyrido[2,3-d]pyridines catalyzed by β-cyclodextrin in aqueous solution using a QM:QM method.

Resumo/Abstract

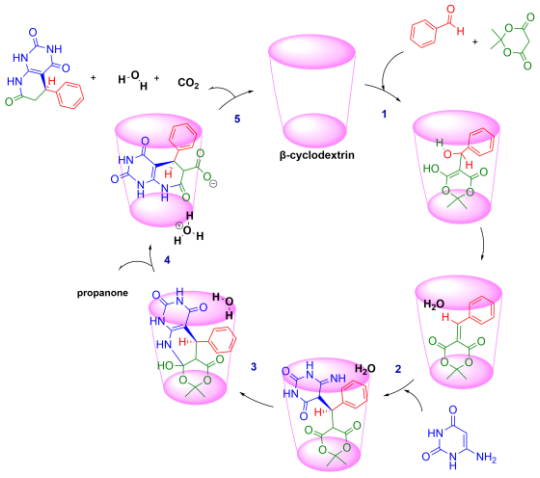
Pyrido[2,3-d]pyridines represent a notable class of heterocycles that contains a pyrimidine core. Given their significant biological activities, developing sustainable synthetic strategies for their production is highly relevant.[1] In 2020, b-cyclodextrin (βCD) was efficiently applied in the synthesis of these compounds in aqueous solution at 100 °C, generating a product with 92% yield.[2] Although the authors proposed a mechanism, there is a lack of theoretical studies to support their hypothesis. The main objective of this work is to provide the molecular elucidation of the multicomponent reaction mechanism for the formation of pyrido[2,3-d]pyrimidine derivatives catalyzed by βCD in aqueous solution. Given that it is a relatively large system, we used a subtractive hybrid QM:QM method, whose combination of high and low levels of theory were X3LYP/def2-SVP:xTB. In this work, we restricted ourselves only to evaluating the encapsulation effect caused by bCD. According to our results, the mechanism follows the same mechanistic steps of the uncatalyzed reaction[3] (**Scheme 1**), however, with different magnitudes of the activation barrier and with the rate-determining step being the protonation of a tertiary carbon by the hydronium ion in the Michael addition mechanism. To our knowledge, this work is the first complete theoretical elucidation of the mechanism formation of pyrido[2,3-d]pyrimidine derivatives catalyzed by βCD in aqueous solution.

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2. Chate, A. V.; Kulkarni, A. S.; Jadhav, C. K.; Nipte, A. S.; Bondle, G. M.*J. Heterocycl.Chem*.**2020**, 57 (5), 2184-2193.

3. Rufino. V. C.; Amarante, G.W.; Dos Santos, H.*ACS Omega*,**2025**, 10, 27393−27403.



Catalytic cycle of β-cyclodextrin catalysis in a multicomponent reaction.

Agradecimentos/Acknowledgments

The authors would like to thank CNPq (173203/2023-0), FAPEMIG and EULER/CeMEAI.

Theoretical study (DFT) of the non-complexation of dithiocarbazate ligands with Ni(II) and Cu(II).

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Palavras Chave:*DFT,dithiocarbazates,transition metals,complexation,rotational activation energies*

Highlights

DFT analysis shows the synthesized dithiocarbazate ligands can thermodynamically bind Ni(II) and Cu(II), but anti N–S conformations create kinetic barriers that prevent complex formation.

Resumo/Abstract

This work presents a theoretical study based on electronic structure calculations to investigate the reasons for the lack of complexation of dithiocarbazate ligands with Ni(II) and Cu(II) ions observed in previous experimental studies. The main motivation lies in the search for new metal complexes with potential chemotherapeutic activity and lower toxicity compared to classical compounds such as cisplatin.

The calculations were carried out within the framework of Density Functional Theory (DFT) using the ORCA 6 program, with the ωB97X-D4 functional and the def2-TZVP basis set, including solvation effects consistent with the experimental conditions. The metals were modeled as chlorides in ethanol, and different coordination geometries and spin states were evaluated.

The results indicate that the formation of the metal complexes is thermodynamically favorable, suggesting spontaneous complexation reactions. Copper complexes tend toward distorted square-planar geometries, while nickel complexes adopt tetrahedral coordination. Variations in the ligand substituents showed only a minor energetic effect.

However, structural analysis reveals that, in the most stable ligand conformation, the sulfur and nitrogen donor atoms adopt an anti orientation, which prevents direct bidentate coordination. Complexation therefore requires rotation of the sulfur atom, indicating that conformational and kinetic barriers, rather than purely thermodynamic factors, are the main reasons for the experimentally observed failure. Future studies will quantify these rotational barriers to fully elucidate the complexation process.

Thermal Stability of Eucalyptus Coal with Potential for Adsorbing Environmental Pollutants

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Palavras Chave:*Coal,Thermal Degradation Kinetics,Thermogravimetric Analysis,Neural Network Modeling,Adsorbent Materials*

Highlights

Thermal Degradation Kinetics of Eucalyptus Coal Evaluated by Thermogravimetry; Multistage Decomposition Process; Variable Activation Energy and Complex Reaction Mechanisms.

Resumo/Abstract

The demand for technologies to remove environmental pollutants has driven the use of coal, whose adsorbent efficiency depends on their physicochemical properties. Thus, the thermal stability of a coal obtained from eucalyptus (Eucalyptus globulus Labill) was evaluated in an experimental phase as an adsorbent of environmental pollutants. The kinetic study of the thermal degradation of this charcoal was performed based on thermogravimetric (TG) curves in air (50 mL min^{-1}) at heating rates of 12, 14, and 16 °C min^{-1} from 30 to 850 °C. The TG curves revealed that the decomposition process occurs mainly between 650 and 830 °C, depending on the heating rate, with the degradation shifting to higher temperatures as the rate increases. Isoconventional analysis revealed that the activation energy (Ea) varies between 72 kJ mol^{-1} (α = 0.1) and 100 kJ mol^{-1} (α = 0.9). This progressive increase indicates the transition to the breakdown of more stable structures. Kinetic modeling by neural networks (MLP) identified the simultaneous contribution of different models, with emphasis on the Avrami-Erofeev nucleation and growth mechanism of order 2 (Am2), which presented the highest normalized contribution and the lowest individual residual error. For the Am2 model, the logarithm of the frequency factor () ranged from 9.8 to 13.8 throughout the conversion, confirming structural and reactive area changes during the process. The results highlight the heterogeneous and multimechanistic nature of the decomposition, with the Am2 model best describing the physicochemical phenomenon involved, providing crucial parameters for the technological optimization of the material.

Agradecimentos/Acknowledgments

The authors would like to thank FAPEMIG and CNPQ for their support.

Unraveling the Kinetics of Cosmic Ray-Induced Chemistry in Astrophysical Ice Analogs via the PROCODA Code

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[1]Universidade do Vale do Paraíba

Palavras Chave:*Chemical Kinetics,Ice Processing,PROCODA,Sputtering,Reaction Pathways*

Highlights

PROCODA models kinetics of irradiated astrophysical ices.
Computational simulations match experimental data.
Reaction rates and sputtering yields are quantified with implications for astrochemistry.

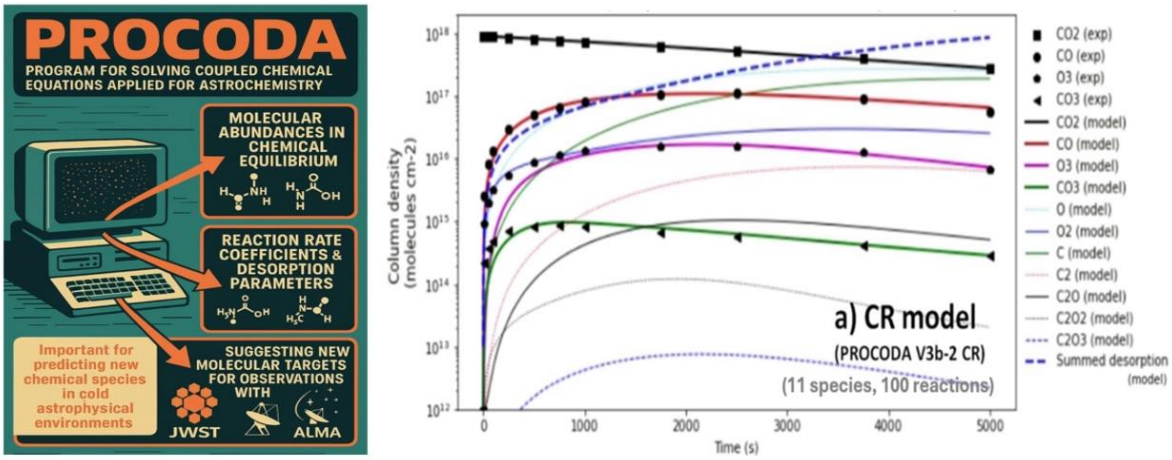
Resumo/Abstract

We present a computational study of the physicochemical evolution of astrophysical ice analogs processed by energetic cosmic ray analogs. Utilizing the Python-based PROCODA code, we model the complex kinetics of ice chemistry in simulated space environments, including cold molecular clouds and planetary surfaces [1,2]. By solving a system of hundreds of coupled differential equations, the model successfully reproduces experimental data for both pure ices (H2O, CO, CO2, and CH4) and binary ice mixtures (H2O:CO2, H2O:O2, H2O:CO, and H2O:HCOOH) [3-7].

This work focuses on quantifying key physicochemical parameters, including bulk reaction rates, radiation-induced desorption (sputtering) yields, and the establishment of chemical equilibrium phases. Furthermore, we map the dominant reaction pathways driving molecular complexity in these ices. The results provide critical insights into the non-thermal processing of condensed matter in space, with significant implications for our understanding of prebiotic chemistry and the astrochemical evolution of star-forming regions.

Keywords: Chemical Kinetics, Ice Processing, PROCODA, Sputtering, Reaction Pathways

References:[1] Pilling S. et al. 2022; ApJ, 925, 147 (original PROCODA paper); [2] Pilling S. et al. 2023a, ASR, 71, 5466 (PROCODA paper with code upgrades); [3] Pilling S. et al. 2023b, MNRAS, 523, 2858 (H2O ice); [4] Gerasimenko S. et al. 2025, MRNAS, 544, 855 (CH4 ice); [5] Silva J. et al., 2025, ApJ, 985, 254 (H2O:O2 ice); [6] Moraes L. et al. 2025, Icarus Submitted. (H2O:CO2 ice); [7] Fargnoli C. et al. 2026, ASR Submitted. (H2O:HCOOH ice)



Some PROCODA code features and a sample of modeling of pure CO2 ice irradiated with ions (ref 1)

Agradecimentos/Acknowledgments

The author acknowledges financial support from the Brazilian agencies CNPq (grant 302608/2022-2) and FAPESP (grant 2024/05115-5).

Unveiling Electromechanical Coupling in Elastomers: Beyond an Obvious Key to Advanced Materials

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Palavras Chave:*Elastomers,Electromechanical coupling,Flexoelectricity,Hygroelectricity*

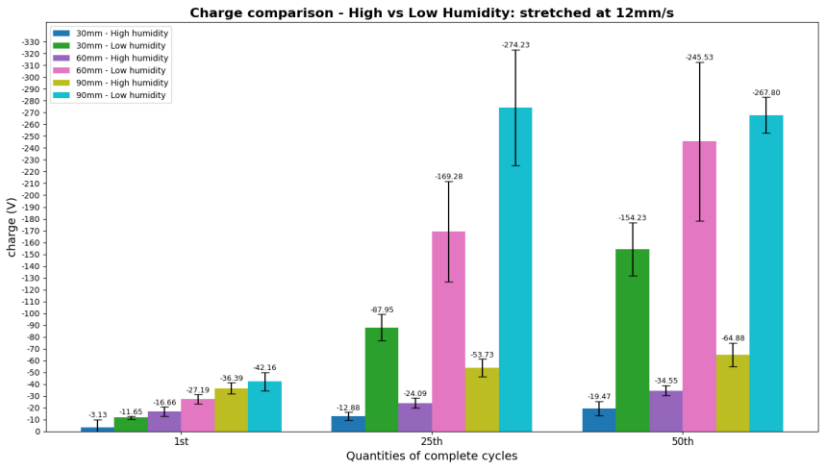
Highlights

Flexoelectricity alone cannot describe electrostatic behavior in elastomers.
Rethinking electromechanical coupling requires accounting for hygroelectricity.

Resumo/Abstract

Elastomers exhibit significant deformation under mechanical stress, making them ideal platforms to study electromechanical coupling mechanisms such as flexoelectricity. These materials can generate electrostatic potentials not only via bond polarization under strain but also through surface charge accumulation influenced by ambient conditions. In industrial environments, understanding these effects is critical, as uncontrolled charge buildup can lead to hazardous discharges or explosions. While flexoelectricity is commonly invoked to explain the voltage generation during deformation, recent evidence suggests that ambient humidity plays a major role in modulating the observed potentials. The asymmetric distribution of water vapor ions and changes in surface conductivity influence the magnitude and polarity of the electrostatic potential. This raises questions about whether flexoelectricity alone is sufficient to describe the observed behavior in elastomers.

To investigate this, we conducted controlled experiments using natural rubber films (10 mm length) subjected to repeated stretching–relaxation cycles. At 12 mm/s, a 30 mm stretch amplitude produced a steadily increasing negative electrostatic potential over 50 cycles. In low humidity (<35%), voltages reached –28.6 V, while in high humidity (>70%) the same protocol yielded only –3.9 V. The evolution of charge with cycle count indicates a memory effect driven by entropy and polymer chain reconfiguration. We consistently observed negative potentials, with their magnitude increasing linearly with humidity level, strain velocity, and stretch amplitude. These findings highlight the importance of environmental conditions in tuning the electromechanical response of elastomers. By decoupling purely mechanical effects from humidity-mediated charge dynamics, this work contributes to the development of reliable flexoelectric materials and smart surfaces for sensing, energy harvesting, and electrostatic control.



Electrostatic potential compared under different humidity and stretching conditions over 50 cycles.

Unveiling the Mechanistic Framework of Electrocatalytic Ammonia Oxidation and Its Nitrite/Nitrate Selectivity by a Mononuclear Copper Complex

João Pedro Costa Sarno Neves (PG)*[1], Joel Leitão Nascimento (PG)[1], Roberto Rivelino de Melo Moreno (PQ)[1], Vitor Hugo Menezes da Silva (PQ)[1], Tiago Vinicius Alves (PQ)[2].

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Palavras Chave:*Ammonia Oxidation,Electrolysis,Catalysis,Computational Chemistry,DFT*

Highlights

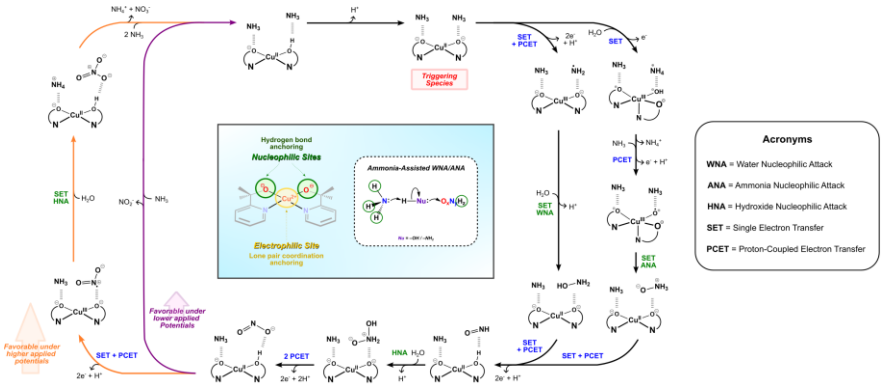
The first N-O coupling is the most relevant to the energy barrier.

Each one is assisted by the ammonia buffer.

The nitrite/nitrate selectivity stems from the last electrochemical activation.

Resumo/Abstract

The electrocatalytic oxidation of ammonia to nitrite and nitrate catalyzed by the mononuclear copper-based complex [Cu(pyalk)$_2$] (pyalk = 2-(pyridin-2-yl)propan-2-oate) has recently demonstrated remarkable electroselectivity (preferential formation of nitrate or nitrite as a function of the applied potential) and chemoselectivity (water*vs*ammonia oxidation as a function of pH) [1]. However, the mechanistic origin of these selectivities has remained unclear. Herein, we provide new insights into the complete electrochemical catalytic cycle of ammonia oxidation (AO) in aqueous media from Density Funcional Theory (DFT) calculations. Our results reveal that the transformation does not proceed through a single oxyl-centered pathway, as previously proposed, but rather through a set of competing electrooxidation-driven sequences that activate the Cu complexes to enable the successive N-O bond formations, the first one being most significant for the energy barrier. New mechanistic scenarios were identified in which the pyalk ligand also serves as an anchoring site for reactive intermediates. In this context, the water directly participates as a nucleophile, and the ammonia buffer plays a crucial role throughout the elementary steps of the catalytic cycle (Figure). The ammonia saturation enables its effective participation in the secondary coordination sphere, promoting key intermolecular interactions that are energetically conducive to N-O bond coupling processes. Finally, we demonstrate that subsequent electrochemical oxidation steps act as the primary driving forces governing the experimentally observed selectivity. Overall, this work establishes an unprecedented mechanistic framework for copper-mediated ammonia oxidation and provides molecular-level insights into the factors that control selectivity in intricate electrocatalytic nitrogen transformations.
[1] Liu, H.*et al.*J. Am. Chem. Soc.**2025**,*147*, 1624–1630.



Proposed catalytic cycle for aqueous ammonia electrooxidation by the complex [Cu(pyclen)2].

Agradecimentos/Acknowledgments

We'd like to acknowledge the funding agencies CAPES, CNPq and FAPESB, as well as the IQ-UFBA and the research group LaTEC-UFBA.

Unveiling the TcP21-CXCR4 Interface: Atomistic Insights into Chagas Disease Pathogenesis

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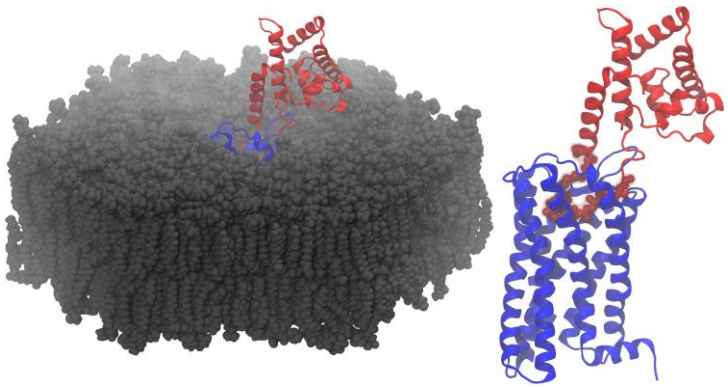
Palavras Chave:*Chagas Disease,GPCR,TcP21,Molecular Dynamics,Interaction Interface*

Highlights

First atomistic model of the TcP21–CXCR4 interface—a key structural trigger for T. cruzi extracellular amastigote infection—via critical consensus-scored, multi-mode, multi-replica MD simulations.

Resumo/Abstract

Chagas disease remains a significant global health burden after more than a century of discovery. Experimental evidence has shifted the infection paradigm, revealing that the "replicative" amastigote form of*T.cruzi*is also highly infective[1]. Central to this is TcP21, a protein secreted by extracellular amastigotes that facilitates host-cell invasion via interaction with the CXCR4 chemokine receptor. However, the structural mechanism governing this interaction remains unknown[2]. We employed an integrated computational workflow to elucidate the TcP21-CXCR4 interaction interface. Following molecular docking to identify plausible cluster-based binding modes (5), we conducted multiple-replica (5) molecular dynamics simulations to assess complex stability. To pinpoint critical interface residues, we applied a multi-metric ΔSASA-based scoring routine integrating independent biophysical metrics into a weighted consensus score. Analysis identified a 16-residue hotspot (residues 23–39) within a disordered loop of TcP21 and 13 residues distributed across the extracellular domain of CXCR4. These regions form a coordinated anchoring network consistent across multiple binding modes and replicas. The interaction is driven by a robust electrostatic network, featuring 15–18 consistent hydrogen bonds and 6–10 salt bridges. Spatial analysis strongly suggests TcP21 occupies the extracellular opening of the receptor, creating a critical steric hindrance that prevents simultaneous binding of the native ligand, CXCL12. This indicates a competitive inhibition mechanism that may disrupt native signaling to facilitate parasite entry. This study provides the first structural proposal for the TcP21-CXCR4 signaling trigger. By defining these key residues, our results offer a mechanistic basis for how*T.cruzi*exploits host CXCR4 for internalization, identifying a high-value target for future therapeutic intervention.
1. ACS Infect. Dis.;2022;8;6;1107–15
2. Front. Cell Dev. Biol.;2020;8;569729



TcP21 (red)–CXCR4 (blue) MD representative complex in lipid membrane. Right: TcP21 interacting loop.

Agradecimentos/Acknowledgments

The authors acknowledge FAPEMIG (Proc. 5.10/2022) for the provided financial support and the Auburn University Computational Biophysical Group for their vital collaboration.

Valorização da Palha de Milho para Síntese de Triacetato de Celulose: Influência da Concentração de Ácido Sulfúrico na Acetilação

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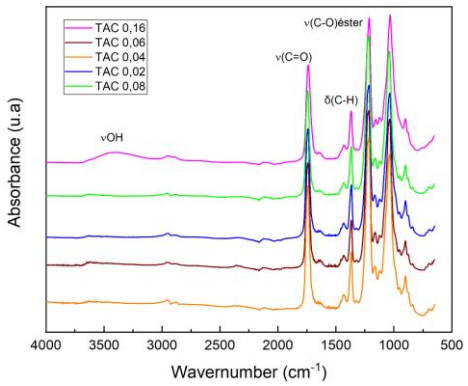
Palavras Chave:*Triacetato de celulose, palha de milho, ácido sulfúrico, massa molecular viscosimétrica média*

Highlights

Corn husk was valued for the synthesis of cellulose triacetate, evaluating the variation in sulfuric acid concentration, with FTIR confirming acetylation and a degree of substitution close to 3.0.

Resumo/Abstract

A palha de milho é um resíduo agrícola, subaproveitado na geração de energia por meio de sua queima ou de sua deposição no solo de plantio, porém, pode ser reaproveitado e processado de forma a agregar valor ao material final. Rica em celulose, com teor de na faixa de 45%, a palha pode ser aproveitada para a síntese de triacetato de celulose (TAC), um polímero termoplástico com amplas aplicações, como membranas em processos de separação, monolitos para remoção de contaminantes ambientais, entre outras. A produção de TAC a partir da celulose extraída da PM foi investigada com ênfase nos efeitos da variação da concentração do catalisador, ácido sulfúrico concentrado, variando de 0,02 a 0,16 mL para 1 g de celulose. O volume de catalisador deve ser reduzido o suficiente para evitar degradação da cadeia celulósica e garantir a modificação química. A caracterização foi realizada por Espectroscopia de Absorção no Infravermelho com Transformada de Fourier (FTIR), evidenciando bandas típicas do TAC, como o estiramento C=O do éster em 1750 cm^{-1}, o estiramento C–H do metil e o estiramento C–O do grupo acetil. Por meio da análise FTIR, foi avaliado o grau de substituição (GS) pelo cálculo das áreas das bandas do TAC e obteve-se um valor próximo de 3,0 para todas as amostras.[1]Este resultado evidenciou que mesmo variando o volume de H_2SO_4, na faixa estudada, não houve prejuízo na produção do TAC, obtendo-se valores médios próximos a faixa de caracterização do polímero em estudo (GS 2,7 a 3,0). Para avaliar o controle da degradação da cadeia polimérica, foi determinada a massa molecular viscosimétrica média (Mv) das amostras estudadas. Observou-se que a amostra preparada com 0,06 mL de H_2SO_4 apresentou o melhor desempenho na preservação das cadeias celulósicas, alcançando uma Mv de 6090,92 $g \cdot mol^{-1}$. Esse resultado indica elevado potencial para aplicação na produção de membranas e monolitos.
[1] J. Wolfs 1; F. C. M. Scheelje; O. Matveyeva; M. A. R. Meier. 2023, 61, 2697.



FTIR das amostras TAC 0,02; 0,04; 0,06; 0,08 e 0,16.

Agradecimentos/Acknowledgments

Ao CNPQ, PROPP, RELAM-UFU, FINEP (INF13 01.130371.00) e a UFU

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Anthraquinone-mediated organic photocatalysis in photoassisted amidation reactions

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[1]Universidade Federal do ABC

Palavras Chave:*Light, Organic dyes, Organic synthesis, Photochemical reaction, Sustainability*

Highlights

Anthraquinone shows promising performance as an organic photocatalyst for photoassisted amidation, outperforming classical dyes and metal complexes.

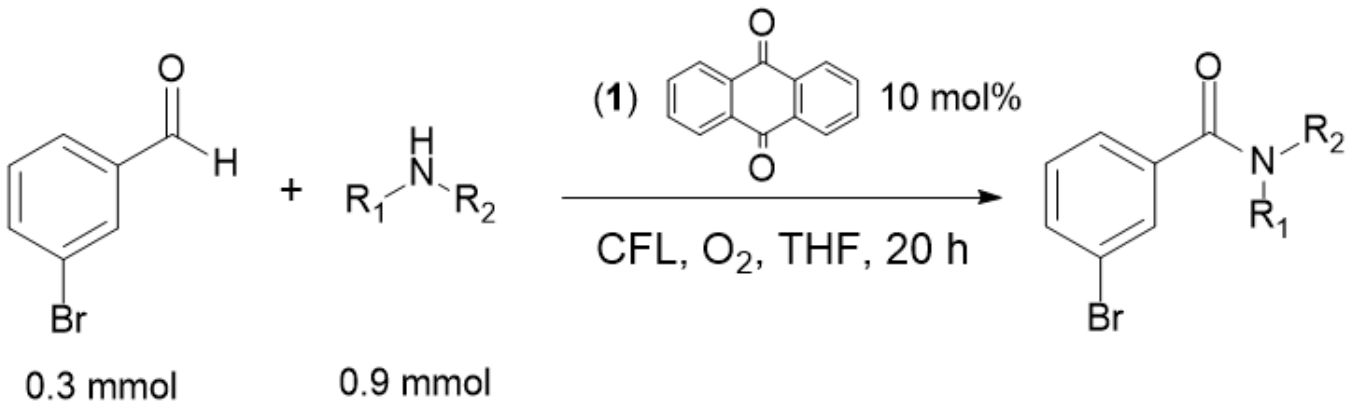
Resumo/Abstract

Anthraquinones (AQs) are an important class of organic dyes whose photophysical and redox properties make them attractive candidates as organic photocatalysts in light-driven transformations [1]. Their high stability, strong absorption in the UV-Vis region, and access to long-lived excited states enable their use as sustainable alternatives to conventional metal-based photocatalysts. Herein, we investigate the use of AQs as organophotocatalysts in photoassisted amidation reactions. We first studied the photophysical properties of five AQs, containing chloro, hydroxyl, sulfonate, and carboxyl substituents, in addition to the parent AQ (1). The absorption maxima are within the 320-430 nm range, with ε >5000 L mol–1; and all AQs presented negligible fluorescence. AQs were then applied as photocatalysts of a model amidation reaction,[2] using m-bromobenzaldehyde as substrate and aniline and pyrrolidine as representative primary and secondary amines, respectively. Reactions were carried out in 5 mL of THF, under O_2-flow and white light irradiation (compact fluorescent lamp), with 0.3 mmol of substrate and 10 mol% of AQ. Preliminary results show efficient formation of the amidation product employing aniline, with 1 as the photocatalyst, affording an isolated yield of approximately 60% after column chromatography (silica gel, Hex:EtOAc 9:1). This yield exceeds those reported for related systems employing classical photosensitizers, such as methylene blue and rose bengal, as well as metal-based, $Ru(bpy)_3Cl_2$ and $Ir(ppy)_3$, which generally provide 20-40% yields [3]. These results underscore the potential of AQs as efficient organic photocatalysts and support their application as simple, accessible, and sustainable alternatives in photoassisted amidation methodologies.

[1] Chen et al. Environ. Sci. Ecotechnol. 2024, 22, 100449.

[2] Inagawa et al. Asian J. Org. Chem. 2019, 8, 1411.

[3] Leow Org. Lett. 2014, 16, 5812.



Agradecimentos/Acknowledgments

Agradeço a UFABC, CAPES e a CEM (Central Experimental Multiusuário da UFABC)

Brooker's Merocyanine-Inspired Solvatochromic Sensors for Pure and Mixed Solvents

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Palavras Chave:*solvatochromic dyes,merocyanines,solvatochromism,reverse solvatochromism,preferential solvation*

Highlights

Novel BM-inspired dyes synthesized. Solvatochromic behavior investigated in 28 pure solvents and water-alcohol mixtures. Negative solvatochromism with borderline reversal in low-polarity media.

Resumo/Abstract

Brooker's merocyanine (**BM**) is a dye widely employed in the study of pure solvents and binary solvent mixtures. Its unusual reverse solvatochromic behavior in solution has motivated the development of related molecular probes. In this work, two new dyes structurally analogous to**BM**were synthesized and characterized. In their deprotonated forms (**1b**and**2b**;**Figure 1**), these compounds exhibited solvatochromism and were applied to assess polarity in pure organic solvents. UV-vis spectra were recorded in 28 different pure solvents, showing marked variations in visible absorption bands. The molar transition energy (*E*T) values were determined and compared with literature data, revealing negative solvatochromism with borderline reversal in low-polarity media. Data analysis using the Catalán approach indicated that medium acidity was the most influential parameter in probe solvation. Furthermore, the dyes were tested in water–alcohol binary mixtures, with*E*T values plotted against water mole fraction. Experimental results were fitted to theoretical curves based on a classical solvent-exchange model within the probe solvation sphere. The observed behavior was interpreted in terms of solute–solvent and solvent–solvent interactions, confirming the applicability of these probes in studies involving binary solvent systems.

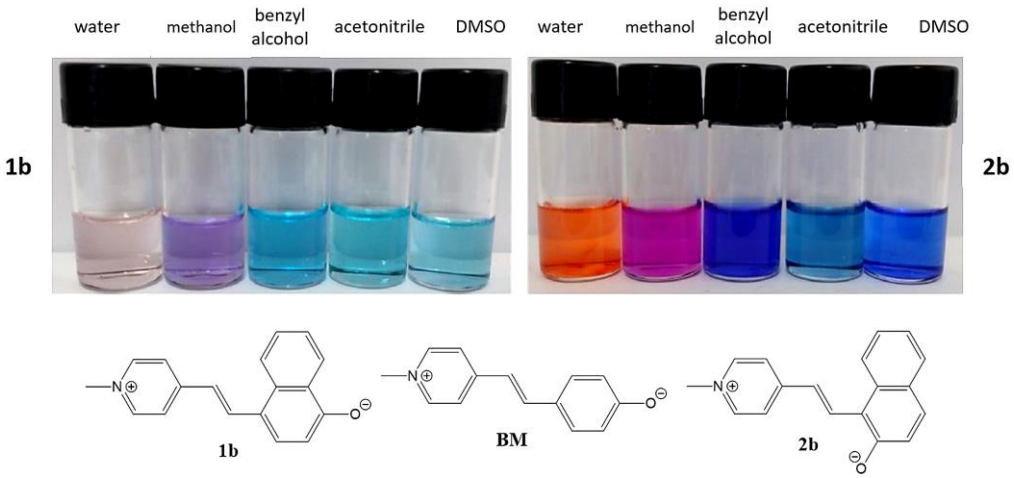


Figure 1. Molecular structures of BM, 1b, and 2b and solutions of the dyes in some selected solvents

Agradecimentos/Acknowledgments

CNPq (Process numbers 407774/2021–1 and 311387/2023-3), Instituto Nacional de Pesquisa e Inovação em Imagem Fototérmica (INPIIF/CNPq; process number 408454/2024-5), CAPES (Finance code 001), and FAPESC (Process number: 2024TR002301).

Designing of a Modular Small-Scale Flow Photoreactor for Affordable Laboratory Photochemistry

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Palavras Chave:*Flow Reactor,DIY,Photochemistry,3D Printing,Accessibility*

Highlights

A low-cost modular flow photoreactor with broad wavelength flexibility (~365–540 nm) is demonstrated as an accessible tool for diverse photochemical applications.

Resumo/Abstract

Photochemical methodologies have gained increasing relevance due to their unique reactivity profiles and compatibility with continuous flow processing. However, access to flow photoreactors remains limited in many small and academic laboratories, particularly in resource-constrained environments, due to the high cost and limited spectral flexibility of commercial systems.

This work presents the design and construction of a**low-cost**,**laboratory-scale modular flow photoreactor**intended to expand access to flow photochemistry across a broad range of excitation wavelengths. The system is based on a custom-built quartz tubing flow cell housed within an internally reflective irradiation chamber and equipped with interchangeable**12W**LEDs modules operating at 365 nm (**UV**), 410 nm (**blue**), 520 nm (**green**), and 590 nm (**yellow**). This spectral range enables compatibility with a wide variety of photocatalysts and photochemical transformations reported in the literature.

Reactor operation and control are managed through an ESP-32–based embedded system with touchscreen interface, allowing adjustment of irradiation parameters and supporting**reproducible**experimental conditions. The modular architecture permits straightforward replacement or upgrading of light sources, facilitating**future scalability**, particularly with respect to LED wattage and optical output.

While photochemical validation reactions were not completed at the time of submission, the reactor was designed with established model reactions in mind. Such as the photo-reduction of**benzophenone**in isopronol for**UV**validation and thephotocatalysis using**pyrene-4-5-dione**for**visible light**validation. Overall, this platform emphasizes**affordability**,**wavelength versatility, and modularity**, providing a practical entry point for flow photochemistry in small research laboratories.



AI generated image of the photoreactor for ilustrative purposes

Design of Phenanthroline-Coordinated Ni(II) Complexes for Radical Photopolymerization

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[1]Faculdade de Ciência e Tecnologia - UNESP, Campus de Presidente Prudente SP; [2]Universidade Estadual Paulista

Palavras Chave:*Nickel,phenanthroline,photocatalyst,photopolymerization,LED irradiation*

Highlights

Synthesis and characterization of new Ni(II) complexes based on phenanthroline compounds as photocatalysts for radical photopolymerization

Resumo/Abstract

Photopolymerization is an advanced technique that enables the synthesis of polymers with well-defined structures and properties using light as an activation source. When polymer chain growth is controlled, this process is known as Controlled Radical Photopolymerization (CRP2). High-performance photocatalysts based on metal structures are being developed for photopolymerization[1,2]. In this study, Ni (II) metal complexes were synthesized to catalyze and control radical photopolymerization reactions. The first step involved synthesizing phenanthroline ligands and their corresponding Ni (II) complexes (Figure 1), followed by full characterization using FTIR, UV-Vis, ^{1}H NMR, and mass spectrometry. FTIR showed a band at 421 cm^{-1} attributed to Ni-N coordination, while the PF_6^- band at 843 cm^{-1}remained unchanged. Small shifts in C=C and C=N stretching bands suggested ligand coordination effects. UV-Vis spectra displayed π→π* transitions for ligands and bathochromic shifts for the complexes, with a new band near 380 nm assigned to metal-ligand charge transfer. ^{1}H NMR confirmed ligand structures, and MALDI-TOF verified the complexes. Photochemical properties were evaluated by fluorescence spectroscopy. Throughout the study, the photochemical properties of the complexes were evaluated as photocatalysts in photoinitiating systems for FRP. Two systems were investigated: phenacyl bromide/EDB and iodonium salt/EDB under LED irradiation (365 and 390–405 nm). The iodonium system showed higher efficiency and promising performance in the FRP of TMPETA. Photolysis studies under LED@365 nm helped propose the mechanism under optimized conditions. Results indicate that some Ni(II) complexes exhibit suitable photoactive behavior to act as efficient photocatalysts in photopolymerization processes.

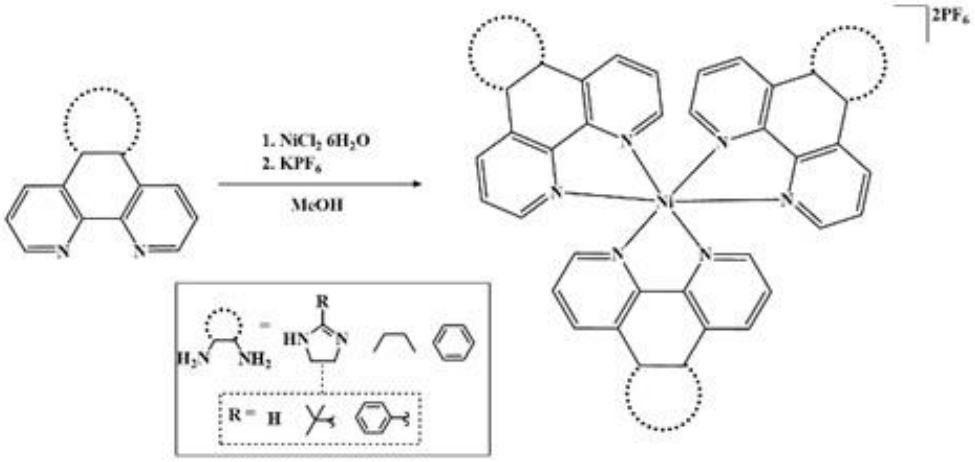


Figure 1. Ni(II) complexes bearing different phenanthroline ligands.

Agradecimentos/Acknowledgments

BEG, VPCJ, NMP are indebted to the financial support from FAPESP, grant #2025/04536-0, grant #2021/13128-1, grant #2021/11741-8, respectively, São Paulo Research Foundation (FAPESP)

Development of Co(II) Complexes Derived from Phenanthroline for Sustainable Applications for Free Radical Photopolymerization.

André Luiz Peres Higuchi (IC)*[1], Yasmin de Morais Shimizo (PG)[1,2], Naralyne Martins Pesqueira (PG)[1], Beatriz Eleutério Goi (PQ)[2], Valdemiro Pereira de Carvalho Junior (PQ)[2].

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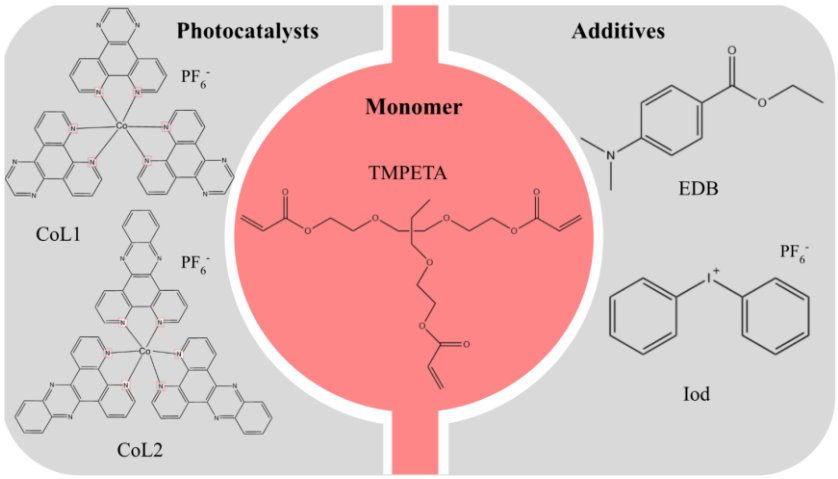
Palavras Chave:*Cobalt,Photopolymerization,Photochemical,LED irradiation,Phenanthroline*

Highlights

Phenanthroline-based Co(II) complexes were investigated as photocatalysts for FRP of TMPETA under 365 and 390 nm LED irradiation, using Iod/EDB as co-initiators, monitored by FTIR.

Resumo/Abstract

The development of sustainable photoinitiator systems for photopolymerization in accordance with the principles of green chemistry, employing visible radiation to provide precise reaction control, lower energy consumption, and milder operational conditions. This light-driven approach represents an environmentally friendly alternative to conventional thermal methods, as it avoids external heating and suppresses the emission of volatile organic compounds, while also offering broad applicability across multiple industrial sectors. The photoinitiators were based on low-cost and earth-abundant cobalt(II) coordination compounds bearing phenanthroline-derived ligands, chosen for their rigidity, bidentate coordination, structural tunability, and favorable photophysical behavior. Their photocatalytic activity was examined in the free radical polymerization of ethoxylated trimethylolpropane triacrylate (TMPETA) under LED irradiation of 365 and 390 nm, with enhanced efficiency achieved through the use of diphenyliodonium hexafluorophosphate (Iod) and ethyl dimethylaminobenzoate (EDB) as co-initiating additives. The methodology comprised the synthesis and comprehensive characterization of ligands and metal complexes, followed by analysis of their spectroscopic, photochemical and photoelectrochemical properties. Polymer formation and kinetic profiles were monitored using FTIR, and structure–activity relationships were established to correlate molecular architecture with initiation efficiency and catalytic performance. By combining sustainable raw materials, non-toxic and biocompatible metals, and light-mediated polymerization strategies, the project contributed to the development of advanced polymeric systems and to a more sustainable cycle of material production and degradation.



All the photocatalyst, addtives and monomers used for photopolymerization reactions.

Agradecimentos/Acknowledgments

Financial support from the São Paulo Research Foundation (FAPESP) under grants #2025/04536-0. São Paulo State University (UNESP), YMS, NMP, IZC and BEG.

DIGA UMA COR E TE DIREI COMO CHEGAR LÁ: UMA MOLÉCULA COM FLUORESCÊNCIA EM QUASE TODO ESPECTRO VISÍVEL A DEPENDER DA FORMA DE CRISTALIZAÇÃO E SOLVENTE

Letícia Develly (PG)*[1], Bruno Dival (PG)[1], Leonardo Pitinato (IC)[1], Willian Xerxes Coelho Oliveira (PQ)[1].

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Palavras Chave:*Luminescência,OLEDs,Solvatocromismo,Polimorfismo,Estrutura cristalina*

Highlights

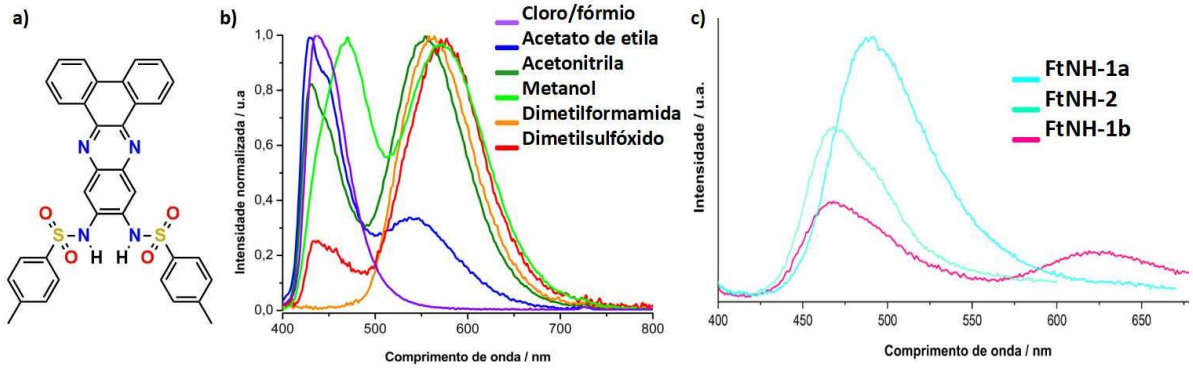
Estudo das propriedades de um material poliaromático (**FtNH**) com fluorescência modulável a partir da polaridade do solvente e da estrutura cristalina, cobrindo larga faixa do espectro de luz visível.

Resumo/Abstract

Materiais luminescentes desempenham papel importante na criação de tecnologias luminosas como os OLEDs , que se destacam pela presença de camada emissiva (metal)orgânica, possibilitando dispositivos mais simples, nítidos e versáteis. Nesse contexto, compostos poliaromáticos destacam-se devido a elevada conjugação π, que aproxima a energia dos orbitais de fronteira e otimiza suas propriedades luminescentes. O composto**FtNH**(Fig. 1a) pertence a esse grupo e apresenta uma parte rígida e aproximadamente plana, composta por cinco anéis aromáticos interligados, mas também uma porção flexível, formada por grupos tosila, com possibilidade de ligação de hidrogênio intramolecular. Essas características estruturais permitem que a fluorescência seja modulada de acordo com o ambiente químico e arranjo espacial da molécula.

Em solução, o**FtNH**apresenta solvatocromismo dependente da polaridade (Fig. 1b). Em solventes menos polares apresenta emissões próxima a região do violeta-azul, enquanto que o aumento da polaridade promove tanto um deslocamento batocrômico, como surgimento de uma segunda banda de emissão. Esta se deve pela transferência protônica intramolecular no estado excitado (ESIPT), com emissões nas regiões do verde, amarelo e laranja. A emissão pode ser finamente ajustada realizando misturas de solventes.

No estado sólido, o comportamento do**FtNH**é dependente do solvente de cristalização e da conformação dos grupos tosilas (Fig. 1c).**FtNH-1a**é anidro e**FtNH-2**um solvato de DMSO. Eles apresentam emissões semelhantes na região do azul, com pequenas variações atribuídas à presença de DMSO em**FtNH-2**que compete pelas ligações de hidrogênio envolvidas no ESIPT. Ao aplicar pressão em**FtNH-1a**obtém-se um polimorfo,**FtNH-1b,**que apresenta mudança estrutural significativa, que reflete em um deslocamento intenso da emissão para a região do vermelho. Esses resultados evidenciam o potencial do composto, destacando o**FtNH**como um material promissor para aplicações optoeletrônicas.



a) Estrutura molecular do FtNH. Emissão b) em solução e c) dos sólidos de FtNH; excitação a 365 nm.

Agradecimentos/Acknowledgments

Agradecimentos aos órgãos de fomento FAPEMIG, CNPq e CAPES pelo suporte financeiro (420443/2018-5, APQ-05311-23, APQ-03469-25, e APQ-01948-22), ao Departamento de Química e LabCri pela infraestrutura para análises.

Evaluation of the Substituent and Solvation Effects on the Photophysical Properties of Tetraphenylimidazoles

Willians Silva Zaguini (PG)*[1], Débora Assumpção Cunha (PG)[1], Leonardo Martins Carneiro (PG)[1], Brenda Fany Rodrigues (PG)[1], Paula Homem-de-Mello (PQ)[1], Fernando Heering Bartoloni (PQ)[1].

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Palavras Chave:*Light,Organic dyes,Organic synthesis,Condensation reaction,LFER*

Highlights

Substituent and solvation effects were investigated to better understand the photophysical properties of tetraphenylimidazole derivatives of interest.

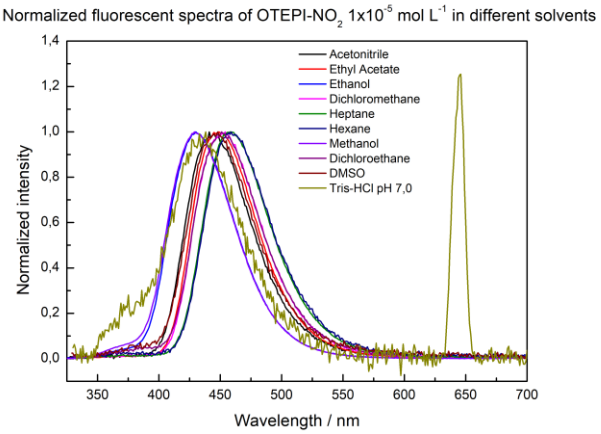
Resumo/Abstract

Substituent and solvation effects are important factors in chemical transformation analysis, influencing reaction rates,[1] mechanistic pathways,[2] and luminescent properties.[3] In this work, we verified the influence of electron-donating and electron-withdrawing groups in the properties of tetraphenylimidazole derivatives. Four derivatives were synthesized and isolated: 1,2,4,5-tetraphenyl-1H-imidazole (TEPI-H), 2-(1,4,5-triphenyl-1H-imidazol-2-yl)phenol (OTEPI-H), and OTEPI-OMe and OTEPI-NO_2 (i.e., the para position at ring 2 contains a methoxy or nitro group, respectively). These derivatives were synthesized through a Debus-Radziszewski reaction. After purification by recrystallization, the compounds were characterized through ^{1}H and ^{13}C NMR. The photophysical parameters were obtained through Uv-Vis absorption and fluorescence spectrophotometry measurements in organic solvents (polar protic, polar aprotic and nonpolar) and Tris-HCl pH 7.0 buffer. Values of maximum absorption wavelength and the associated molar extinction coefficient, maximum fluorescence wavelength, Stokes shift (Δλ), and fluorescence quantum yield (ΦFL) were determined. Overall, Δλ decreases with solvent polarity, with bigger shifts seen in nonpolar solvents (H 15000 cm^{-1}, OMe 13500 cm^{-1}, NO2 12700 cm^{-1}) compared to smaller shifts in polar protic solvents (H 12900 cm^{-1}, OMe 12600 cm^{-1}, NO2 11200 cm^{-1}). Also, ΦFL increases in higher-polarity organic solvents and with the electron-donating group, with values spanning from 19 to 44%. There is, however, a substantial decrease in aqueous buffer for ΦFL, from 88 to 2%, when comparing OTEPI-H and -OMe, respectively.

1. El Seoud, O.A., Baader, W.J. and Bastos, E.L. (2016). Practical Chemical Kinetics in Solution. In Encyclopedia of Physical Organic Chemistry (eds Z. Wang, U. Wille and E. Juaristi).

2. Zhu et al. Phys. Chem. Chem. Phys., 2025, 27, 2473

3. Wang et al. Spectrochim. Acta A Mol. Biomol. Spectrosc. 2024, 321, 124714



Normalized fluorescence spectra of OTEPI-OMe for the solvent series

Agradecimentos/Acknowledgments

UFABC, CEM-UFABC, CAPES and FAPESP.

Exploring the Substituent Effect on Excited-State Intramolecular Proton Transfer in Hydroxyaryltriazole Derivatives

Brenda Fany Rodrigues (PG)*[1], Diêgo Ulysses Melo (PQ)[2], Leonardo Martins Carneiro (PG)[1], Paula Homem-de-Mello (PQ)[1], Fernando Heering Bartoloni (PQ)[1].

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[1]Universidade Federal do ABC; [2]Universidade Federal Fluminense

Palavras Chave:*Light, Organic dyes, Organic synthesis, ESIPT, DFT.*

Highlights

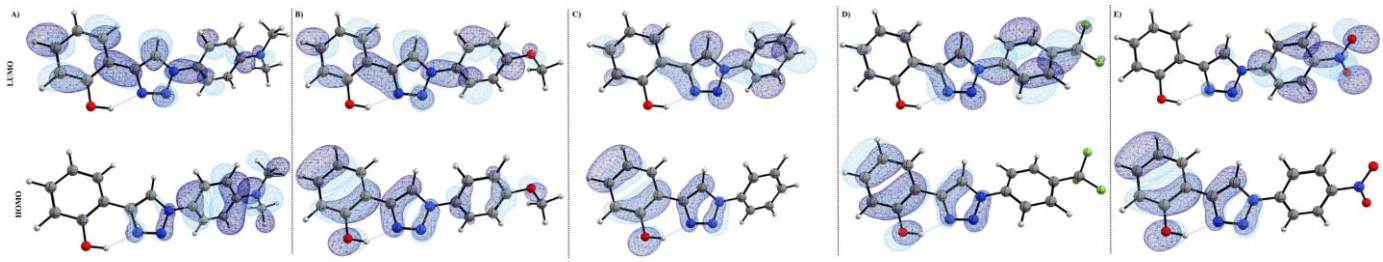
DFT/TD-DFT studies show ESIPT in hydroxyaryltriazoles with EDG/EWG substituents; NMe_2, OMe, H, and CF_3 undergo ESIPT, while NO_2 exhibits charge-transfer character.

Resumo/Abstract

Synthetic organic chemistry is a source of desirable chemical compounds exhibiting photophysical properties, especially conjugated heterocyclic systems such as triazole, a five-membered nitrogen-containing heterocycle conveniently synthesized via click chemistry.[1] Some triazoles are subjected to a particular photophysical mechanism called excited-state intramolecular proton transfer (ESIPT), in which an enolic species tautomerizes to a ketonic one in the excited state, leading to highly desired effects.[2] Furthermore, ESIPT could be affected by the presence of different substituents, related to electron-donating (EDG) or electron-withdrawing groups (EWG). Herewith, we studied the synthesis and explored ESIPT in a series of hydroxyaryltriazole derivatives containing different substituents, including EDG and EWG: NMe_2, OMe, H, CF_3, and NO_2.

Preliminary computational studies were performed applying Density Functional Theory (DFT) and Time-dependent DFT (TD-DFT). The CAM-B3LYP hybrid functional and def2-TZVP basis sets were used, and the solvent effect was considered using the Conductor-like Polarizable Continuum Model (CPCM).[3] ESIPT is supported by an analysis of the dihedral angles for NMe_2, OMe, H and CF_3 derivatives, showing there is a change in the molecule geometry caused by the proton transfer. For the NO_2 derivative, there is an indication of stabilization through resonance, thus preventing ESIPT. Additionally, there is a decrease in the dipole moment going from EDG to EWG. The frontier molecular orbitals for the ground state demonstrate localized and charge-transfer (CT) transitions for NMe_2, OMe, H, and CF_3 substituents, although only the CT transition occurs with NO_2. Computational analysis confirmed that most triazole derivatives undergo ESIPT, except the NO_2-substituted compound, which shows charge-transfer character.

[1]Salma et al.*J.Mol.Struct.***2024**,*1301*, 137240; [2]Carneiro et al. J.*Phys.Chem.B***2022**,*126*, 7373; [3]Yanai et al.*Chem.Phys.Lett.***2004**,*393*, 51.



HOMO and LUMO frontier molecular orbitals for the ground state: A) NMe2;B) OMe C) H, D) CF3, E) NO2.

Agradecimentos/Acknowledgments

UFABC, CAPES, FAPESP, Finep, CNPq, CCM, CEM and INCT.

Facile Modification of Multi-Resonance Acceptors and Donors in Intramolecular TSCT-TADF Emitters for OLEDs: A Computational Study

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[1]Universidade Federal Fluminense; [2]Universidade Federal do Rio de Janeiro

Palavras Chave:*Through-space charge transfer; multi-resonance acceptors; TADF; OLED; Intramolecular interactions;*

Highlights

This study highlights the photophysical properties of eighteen TSCT-TADF emitters based on A–S–D configurations have been theoretically investigated using DFT and TD-DFT calculations.

Resumo/Abstract

Through-space charge transfer (TSCT) has attracted considerable interest in the development of thermally activated delayed fluorescence (TADF) emitters. In this study, a series of eighteen TSCT-TADF molecules were designed and investigated using density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The molecular frameworks are designed with phenyl and pyridine core scaffolds, featuring a range of donor units, including carbazole (Cz), diphenylamine (DPA), and dimethylacridine (DMAC). A tert-butyl carbazole (tCz) group was employed as a linker, and organoboron multi-resonance (MR) acceptors incorporating heavy atoms such as oxygen (OB), sulfur (OBS), and selenium (OBSe) were employed to explore their effects on the photophysical and electronic properties of the molecules. These TSCT-TADF molecules exhibit a small interplanar distance, weak intramolecular interactions, and distinct TSCT characteristics. The integration of MR acceptors and potent electron donors markedly influences the excited-state properties, facilitating a small ΔEST, enhanced spin–orbit coupling (SOC), rapidk_r,k_{ISC}andk_{RISC}rates. Through comprehensive computational analysis, it is demonstrated that the incorporation of heavy atoms (OBS & OBSe) into the MR-acceptor, combined with phenyl diphenylamine (PDPA) and phenyl dimethylacridine (PDMAC) donors, underscores their potential for highly promising TSCT-TADF emitters. These findings not only substantiate the viability of these molecular architectures as efficient TSCT-TADF emitters but also delineate a comprehensive design paradigm for the development of next-generation TSCT-based molecules, offering significant potential for the advancement of high-performance organic light-emitting diodes (OLEDs).

Agradecimentos/Acknowledgments

S. Nathiya, M. Panneerselvam and L. T. Costa, thanks for the Computing Resources from Feynman, DIRAC, and CENAPAD Server.

Factorial optimization of GaPc-loaded PLGA-PEG nanoparticles preserved Trp photooxidation kinetic and showed a strong photocytotoxicity in AGS cells

Mateus Souza Alvarenga (PG)[1], Alexia Braga França Teixeira (IC)[2], Manuela Falcon de Carvalho (IC)[2], Lucas Pereira Fabris (IC)[1], Jairo Pinto de Oliveira (PQ)[1], André Romero da Silva (PQ)*[2].

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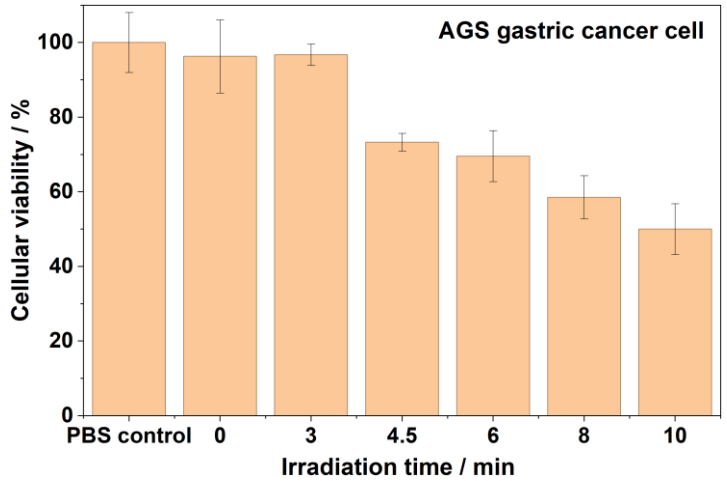
Palavras Chave:*Gallium phthalocyanine,Biomolecule photooxidation,Tryptophan,AGS cancer cell,PLGA-PEG nanoparticle*

Highlights

Poloxamer and stirring rate increased GaPc entrapment efficiency. Encapsulation maintained Trp photooxidation kinetic comparable to free GaPc. GaPc-loaded nanoparticle reduced AGS cancer cell viability.

Resumo/Abstract

Metallophthalocyanines are widely used photosensitizers in photodynamic therapy (PDT). Heavy atoms such as gallium enhance singlet oxygen generation by increasing spin–orbit coupling and intersystem crossing. However, their low solubility limits biomedical applications. To solve this problem, gallium phthalocyanine (GaPc) was encapsulated into PLGA-PEG nanoparticles. A 2^3 factorial design evaluated the effects of polymer mass, Poloxamer 188 mass, and stirring rate on particle size, encapsulation efficiency (EE), recovery efficiency (RE) and zeta potential. Tryptophan (150 µmol/L) in phosphate buffer with Tween 20 (1% v/v) was irradiated in the presence of free or encapsulated GaPc using 665 nm and 638 nm lasers (104 mW). The ability of GaPc-loaded nanoparticles to reduce AGS gastric cancer cell viability was also assessed. Increasing stirring rate and Poloxamer mass raised EE by 5.2% and 5.1%, respectively, with an additional binary synergistic effect. Poloxamer increased zeta potential (2.73 mV), while stirring rate decreased it (2.68 mV). PLGA-PEG mass reduced RE by 4.4%. The Trp photooxidation rate constants for free GaPc were similar at 665 nm (1.4×10^{-4} s^{-1}) and 638 nm (1.3×10^{-4} s^{-1}), but decreased by 47.8% in methylpyrrolidone due to the GaPc photobleaching. Encapsulated GaPc showed a similar rate constant (1.7×10^{-4} s^{-1}) of Trp photooxidation. GaPc-loaded nanoparticles reduced AGS cell viability by 59% after 6 min of irradiation. Encapsulation preserved GaPc photodynamic activity to phooxidate Trp and enhanced its capacity to reduce the viability of AGS cells, demonstrating a promising strategy for metallophthalocyanines.



Photooxidation of AGS cancer cells after a incubation of 2h with GaPC-loaded PLGA-PEG nanoparticle

Agradecimentos/Acknowledgments

We thank CAPES, FAPES (grants 2025-6J1M6H and 2025-CDTT2K), Instituto Federal do Espírito Santo and Universidade Federal do Espírito Santo for financial support for this work.

Iron(II)–NHC Photocatalysts for Advanced Free-Radical, Controlled, and Interpenetrating Network Polymerizations

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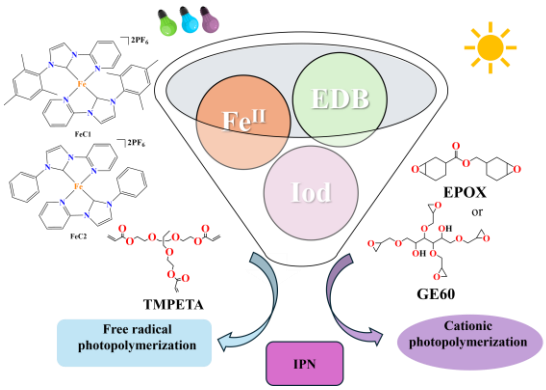
Palavras Chave:*biobased monomers,Fe(II),IPN,FRP,CP*

Highlights

Iron(II) pyridine-NHC complexes are presented as efficient dual photocatalysts for sustainable polymer synthesis. They drive both free-radical and cationic photopolymerization and 3d printing patterns

Resumo/Abstract

The replacement of rare-metal photocatalysts with sustainable, earth-abundant alternatives is a pivotal challenge for green polymer science and advanced manufacturing. This study addresses this need by introducing two novel iron(II) complexes,**FeC1**and**FeC2**(Figure 1), featuring bidentate pyridine–NHC ligands, as highly efficient dual photocatalysts for both free-radical (FRP) and cationic photopolymerization (CP). Their synthesis from $FeCl_2$ and corresponding ligand salts yielded well-characterized complexes with absorption up to 500 nm.Under low-intensity visible light (LEDs at 395, 405, 455, and 532 nm) and crucially under sunlight irradiation, these complexes demonstrated exceptional performance in air and in thick samples (1.8 mm). In the FRP of ethoxylated trimethylolpropane triacrylate (TMPETA),**FeC2**achieved 89% conversion in just 100 seconds at 405 nm. For CP, FeC1 outperformed**FeC2**, reaching a remarkable ~98% epoxide conversion under 405 nm laser irradiation. The scope was successfully extended to biobased monomers (GE60, SARBIO 7201), proving the system's versatility for renewable feedstocks. A significant achievement was the synthesis of interpenetrating polymer networks (IPNs) from blends of TMPETA:EPOX (reaching 60% epoxide conversion) and, notably, from the fully biobased blend TMPETA:GE60, which achieved ~40% conversion even under direct sunlight. Mechanistic investigations via fluorescence quenching, steady-state photolysis, and EPR spectroscopy revealed a preferential oxidative quenching pathway with iodonium salt (Iod), generating aryl radicals for efficient initiation, though involvement of EDB-derived radicals was also detected. This mechanistic insight underpins the high catalytic activity. Finally, translating this chemistry to advanced manufacturing, both complexes enabled high-resolution DLW, fabricating precise 3D microstructures. This work conclusively establishes**FeC1**and**FeC2**as versatile, high-performance, and sustainable photocatalysts.



Summary of the reactions and structures of the compounds used in the reactions

Agradecimentos/Acknowledgments

FAPESP Proc: 25/04536-0, 22/16571-6, 24/03026-5

Lab-on-a-molecule based on a three-site fluorogenic chemical optical device simultaneously detects K+, cysteine, and H+

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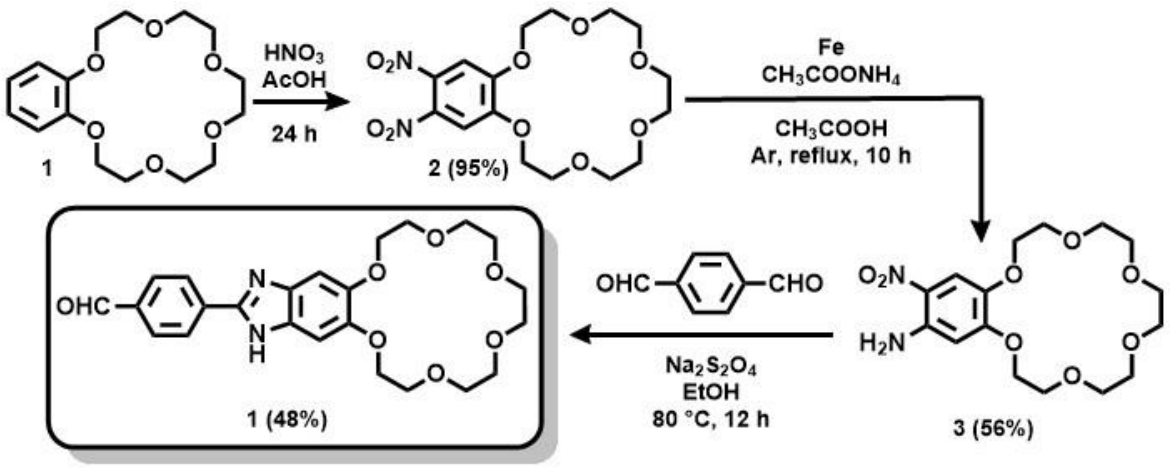
Palavras Chave:*Lab-on-a-molecule, fluorogenic chemosensors, molecular logic gates, functional materials,Lab-on-a-molecule,fluorogenic chemosensors,molecular logic gates,chemodosimeters,functional materials*

Highlights

Compound**1**detects Cys, K^+, and H^+. AND (lab-on-a-molecule) and INHIBIT logic gate operations. Selective recognition of $K^+$and efficient pH sensing.**1**acts as chemosensor and chemodosimeter.

Resumo/Abstract

Fluorogenic chemical optical devices responsive to analytes typically combine a receptor unit and a fluorophore, enabling logic operations where analytes act as inputs and fluorescence signals as outputs. Supramolecular chemistry has refined these concepts, particularly in systems with multiple receptors capable of recognizing more than one chemical species. More advanced devices, termed lab-on-a-molecule, integrate diverse laboratory functionalities into a single structure by detecting three or more analytes simultaneously. Here, we report a new fluorogenic optical device (**1**) with three interaction sites, capable of detecting Cys, K^+, and H^+ through distinct fluorescence responses. Compound**1**incorporates an 18-crown-6 ether for selective cation recognition, especially K^+, and an aldehyde group conjugated with a benzimidazole fluorophore, functioning both as an electron acceptor in intramolecular charge transfer and as a reactive subunit for binding anions or neutral molecules. Compound**1**was synthesized in three steps (**Scheme 1**) and fully characterized by IR, NMR, and HRMS. The device discriminates K^+ among cations, detects Cys within a series of amino acids, and acts as an efficient pH sensor. Logic operations were demonstrated, including AND (lab-on-a-molecule) and INHIBIT gates, using K^+, H^+, and Cys as inputs. Interestingly,**1**shows dual behavior in its aldehyde interactions: acting as a chemosensor for bisulfite and a chemodosimeter for Cys. These findings highlight the versatility of**1**and suggest its potential integration with polymers, fibers, nanoparticles, or other solid supports, paving the way for advanced supramolecular systems in visual and quantitative analyte detection.



Scheme 1. Synthesis of compound 1.

Agradecimentos/Acknowledgments

CNPq (Process numbers 407774/2021–1 and 311387/2023-3), Instituto Nacional de Pesquisa e Inovação em Imagem Fototérmica (INPIIF/CNPq; process number 408454/2024-5), CAPES (Finance code 001), and FAPESC (Process number: 2024TR002301).

"SYNTHESIS OF PHENANTHROLINE-BASED Iron(II) COMPLEXES AS POTENTIAL PHOTOCATALYSTS IN FREE RADICAL PHOTOPOLYMERIZATION REACTIONS"

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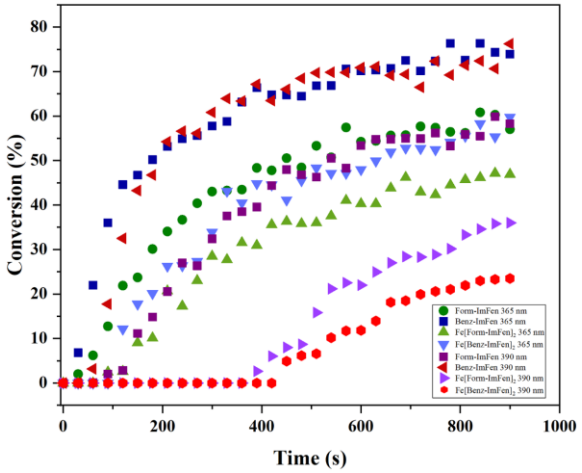
Palavras Chave:*Iron(II) complexes,Photopolymerization,Phenanthroline derivatives*

Highlights

Iron(II)-based photocatalysts were developed for radical photopolymerization, offering a sustainable low-cost alternative to noble metals under light irradiation.

Resumo/Abstract

Free radical photopolymerization (FRP) is a sustainable and energy-efficient technology widely applied in the production of polymeric materials. However, photocatalysts based on noble metals such as ruthenium and iridium present high cost and toxicity, motivating the search for alternatives based on abundant and less toxic metals such as iron. In this work, phenanthroline-derived ligands (R-ImFen) containing two different aldehyde substituents, benzaldehyde (Benz-ImFen) and formaldehyde (Form-ImFen), were synthesized via condensation of 1,10-phenanthroline-5,6-dione with the respective aldehydes, followed by coordination with Iron(II) to obtain the corresponding complexes. The compounds were characterized by UV–Vis, NMR and infrared spectroscopy, confirming the formation of the ligands and the coordination of iron through nitrogen donor atoms, with characteristic spectroscopic changes. Photocatalytic performance was evaluated in systems containing Trimethylolpropane ethoxylate triacrylate (TMPETA) as the monomer, Ethyl 4-(dimethylamino)benzoate (EDB) as electron donor and Phenacyl bromide (PBr) as electron acceptor, under irradiation at 365 and 390 nm. Polymerization kinetics were monitored by real-time Fourier Transform Infrared (FTIR) spectroscopy. The Benz-ImFen ligand exhibited the highest polymer conversion, reaching up to 74% at 365 nm, while Form-ImFen showed moderate activity. In contrast, the Iron(II) complexes presented lower efficiency under the studied conditions, likely due to reduced electron transfer capability after coordination. These results demonstrate the influence of ligand structure on photocatalytic performance and highlight the potential of iron-based systems as sustainable and accessible alternatives for photopolymerization processes.



Polymer conversion of R-ImFen ligands and Iron(II) complexes under 365 and 390 nm irradiation.

Agradecimentos/Acknowledgments

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Light-Driven UV-Visible Photopolymerization and 3D Printing Enabled by Nickel Schiff Base Complexes

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Palavras Chave:*nickel,Schiff base,polymer,LED,3D patterns*

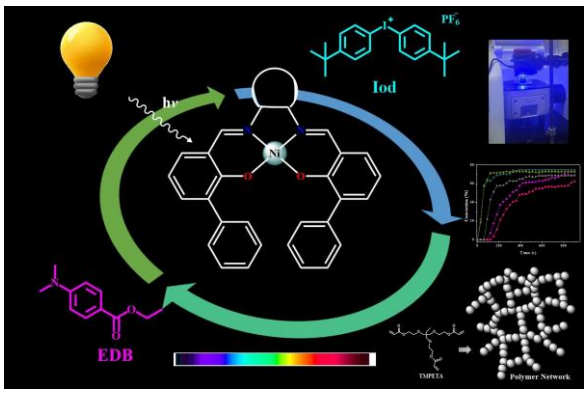
Highlights

Nickel Schiff base complexes were developed as visible-light photocatalysts. Nickel photocatalysts offer a viable alternative to noble-metal systems for photopolymerization and 3D application.

Resumo/Abstract

The development of photocatalysts based on 3*d*transition metals has expanded considerably, particularly for photopolymerization processes relevant to coatings, odontology, nanotechnology, and 3D/4D printing[1]. Among these metals, nickel has attracted attention due to its abundance, stability, low cost, and versatile coordination chemistry[1]. In this work, two nickel complexes bearing symmetrical Schiff base ligands (**NiII-Salen**and**NiII-Salophen**) were synthesized and fully characterized by FTIR, UV-vis, NMR, and ESI mass spectrometry. Their photocatalytic performance was evaluated in free-radical photopolymerization of ethoxylated trimethylolpropane triacrylate (TMPETA), biodegradable monomer, using an iodonium salt, di-tert-butyl-diphenyl iodonium hexafluorophosphate (Iod), as electron acceptor and ethyl 4-(dimethylamino)benzoate (EDB) as electron donor under UV and visible LED irradiation (Figure 1). Monomer conversion was monitored by FTIR through the decrease of the C=C stretching band at 1636 cm–[1]using polypropylene film, without prior oxygen removal. Under optimal conditions, the**NiII-Salophen**exhibited higher overall conversions (>70%) than**NiII-Salen**. The results demonstrate that photocatalytic efficiency is influenced by the ligand framework, particularly the diamine backbone, as well as by the irradiation wavelength. Mechanistic investigations based on photolysis, fluorescence quenching, and ESR spectroscopy support a light-driven redox cycle involving Ni(II)/Ni(III) species, with EDB acting as an electron donor. Thermal analyses (TGA and DSC) and successful application in 3D fabrication further highlight nickel-based photocatalysts as promising alternatives to noble-metal systems for photopolymerization.

[1] N. M. Pesqueira, F. Morlet-Savary, M. Schmitt, V. P. Carvalho-Jr, B. E. Goi and J. Lalevée,*Eur Polym J*,**2024**,*216*, 113279.



"Ni(II)-based three-component photoinitiating systems for TMPETA photopolymerization

Agradecimentos/Acknowledgments

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Microwave-assisted synthesis of carbon quantum dots for photocatalytic applications

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Palavras Chave:*pontos quânticos de carbono, micro-ondas, fotocatálise, hidrogênio, índigo carmim,pontos quânticos de carbono,micro-ondas,fotocatálise,TiO2*

Highlights

Microwave-assisted green synthesis of carbon quantum dots.

Sensitization of TiO_2 under visible light.

H_2 production and pollutant degradation.

Resumo/Abstract

The search for sustainable synthesis routes has highlighted microwave-assisted technology (MWAC) due to its homogeneous heating and high energy efficiency, minimizing undesired thermal gradients. In this scenario, carbon quantum dots (CQDs) emerge as a promising new class of nanomaterials (<10 nm), offering biocompatibility, low toxicity, low cost, and tunable optical properties. When coupled with traditional semiconductors such as TiO2, CQDs act as photosensitizers, extending catalytic activity into the visible light region. This work aimed at the synthesis of copper-doped CQDs via MWAC, using glycerol as a solvent and cupric sulfate (CuSO4) as a reaction promoter. Structural characterization by transmission electron microscopy (TEM) revealed the formation of spherical nanostructures with a mean diameter of 2.7 ± 0.1 nm and (100) crystal planes typical of graphitic structures. Fluorescence spectroscopy indicated maximum emission at 475 nm (390 nm excitation), demonstrating high temporal stability with 90% retention of luminescent intensity over time. For functional evaluation, composites were prepared by impregnating CQDs onto commercial TiO2 (P25) in different mass ratios. Under UV/Vis irradiation from a 140W Xe/Hg lamp, the presence of CQDs significantly increased gas production. The optimized ratio of 1:0.5 (P25:CQDs) reached maximum rates of 90.64 µmol/g·h for O2 and 7.18 µmol/g·h for H2. The observed stoichiometric discrepancy suggests parallel processes, such as the oxidation of oxygenated functional groups on the CQDs' surface. Additionally, to validate the activity exclusively under visible light (λ≥400 nm), the photodegradation of Indigo Carmine (IC) dye was performed. While pure TiO2 proved inactive in this energy range, the Cu-CQDs@P25TiO2 heterojunction promoted total discoloration in less than 3 hours. The kinetics followed the Langmuir-Hinshelwood model, with an apparent rate constant of 6.87×10−3 min−1. These data confirm that the degradation is mediated by electron injection from excited CQDs to the TiO2 conduction band, validating the material as an efficient bifunctional system for both energy conversion and environmental remediation.

Agradecimentos/Acknowledgments

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New Niobium Pentoxide-based Photocatalyst Composites for Visible Light-driven Hydrogen Production by Water Splitting

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Palavras Chave:*Niobium oxide, Non-Noble metal composites, Decoloration,Niobium pentoxide,Non-noble metal composites,Water Splitting,Decoloration*

Highlights

New niobium composite photocatalysts were obtained by Nb2O5 surface decoration, increasing its visible light activity in Rhodamine B decomposition hydrogen production by water splitting.

Resumo/Abstract

Niobium-based materials have been described as promising photocatalysts in the search for sustainable solutions for chemical processes, such as hydrogen production by water splitting.1 Nevertheless, the most common niobium precursors, Nb2O5, have large band gaps and thus are often active under ultraviolet radiation only. Considering this scenario and that Brazil is the leading niobium producer in the world, the present work focuses on tuning the absorption of niobium pentoxide materials towards the visible region to obtain promising sunlight-active photocatalysts for the water splitting reaction.
Organometallic colloids were prepared using low-cost copper or aluminum salts and innocuous organic compounds, and then deposited onto different Nb2O5 samples.
Characterization data indicated that the surfaces of all Nb2O5 precursors could be impregnated with the colloids, as observed by sharp increases in the visible light absorption capacity and the reduction of band gaps to 2.47 eV or lower (> 501 nm).
The materials' photocatalytic activities were initially tested in the decomposition of Rhodamine B in aqueous medium using a 100 W white LED. Dye decomposition upon light exposure was enhanced in the presence of the composites, with catalytic effects up to ca. 10-fold, in comparison to the effects promoted by the pristine oxides, with the composite featuring aluminum and Nb2O5 rich in monoclinic phase deliverying the best results.
After screening the catalysts in the dye decolorization, the best catalyst was selected for H2 production assessment, achieving 50.61 µmol/L at standard conditions, with this value improved to 266.84 µmol/L by optimizing the colloid/oxide ratio along with methanol addition as a sacrificial agent. These results highlight the Nb2O5 catalyst capacity for visible light-induced hydrogen production by water splitting, throughout its modification with environmentally friendly substances, low cost synthesis and decoration with non-noble metals.

Agradecimentos/Acknowledgments

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One pot hydrothermal synthesis of ZnO/MoS2 photocatalyst for dye degradation and H2 production

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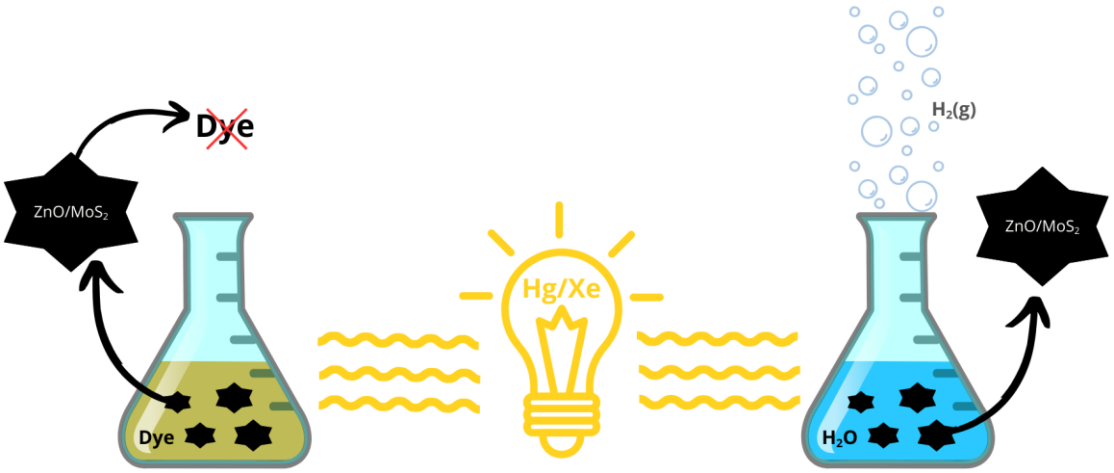
Palavras Chave:*Photocatalysis,Water Splitting,Nanoparticles,Photodegradation,One pot synthesis*

Highlights

One pot synthesis of ZnO/MoS_2 photocatalyst. Photocatalysis for water splitting without noble metals. Photodegradation of ionic dyes.

Resumo/Abstract

In the present days, global warming and pollution caused by fossil fuels demands new and cleaner ways to produce energy. Furthermore, industrialization increases the need for treatment of polluted waters. Our research aimed at nanostructured ZnO/MoS_2 photocatalysts as an answer to these problems based on the vast literature on the topic. The nano structured photocatalyst was obtained via one pot hidrothermal synthesis at 160 oC for 24 h and characterized by several techniques, such as XRD, Diffuse UV and XPS. The photocatalytic properties were first evaluated by photodegrating Methyl Orange and Methylane Blue under a 80 W Hg/Xe lamp. The results of degradation tests were at a rate of 2.53 mg of dye.(g of catalyst)$^{-1}$.h^{-1} and 3,45 mg of dye.(g of catalyst)$^{-1}$.h^{-1} respectively. The results indicate possible photocatalytic activity for H_2 gas production through water splitting, which will also be evaluated in the future. For the time being the synthesized product presents great potential for clean energy production and water decontamination of ionic dyes.



Representation of photocatalysis by ZnO/MoS2 for water splitting and dye degradation

Agradecimentos/Acknowledgments

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Opportunities of MANACÁ beamline at Sirius for the Brazilian chemistry community

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Palavras Chave:*Photocrystallography,Photoisomerization,Serial Crystallography,Synchrotron,Phase Identification*

Highlights

The use of photocrystallography as a tool for the investigation of photoisomerization. Application of serial crystallography for the study of mixture of substances and crystalline phases.

Resumo/Abstract

MANACÁ (**MA**cromolecular micro- and**Na**no-Serial**C**ryst**A**llography) is the Sirius beamline dedicated to the structural determination of macromolecules and is also suitable for crystallographic studies of organic and inorganic compounds, attending the needs of the chemistry community. Recent developments at MANACÁ include the implementation of photocrystallography[1] and serial crystallography[2]. Photocrystallography enables the structural characterization of metastable species and excited states generated under light irradiation[1], while serial crystallography, which is used for microcrystals and time-resolved experiments[3], remains poorly explored for organic and inorganic compounds[4]. In addition, a fragment-screening platform is under development, addressing both macromolecular and medicinal chemistry applications.

In this work, we present results obtained from photocrystallography and serial crystallography experiments at MANACÁ for structural studies. Using photocrystallography, we observed the photoisomerization of [Pd(Bu_4dien)(η^1-NO_2)]BPh_4, reproducing literature conditions[5], revealing the nitro-to-nitrito conversion (**Figure 1**). Showing the capability of MANACÁ for studying light-induced structural transformations. Moreover, serial crystallography was applied to a mixture of alanine and cysteine crystals, allowing the successful solution of both structures and the determination of the absolute configuration of L-cysteine. These results demonstrate the potential of serial crystallography for the characterization of mixed crystalline substances and phases.

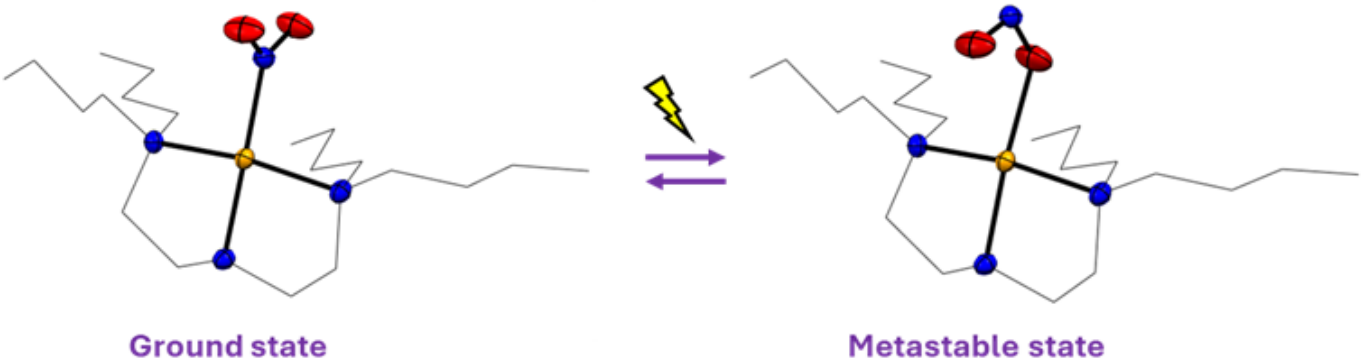
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Single-crystal X-ray structure for the ground state and metastable state

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Opposite-Sign Circularly Polarized Luminescence from Spin-Selective Energy Transfer in Mn-Doped Chiral 2D Perovskites

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Palavras Chave:*CPL,Chirality,2D Hybrid Perovskites,Energy Transfer,TD-DFT*

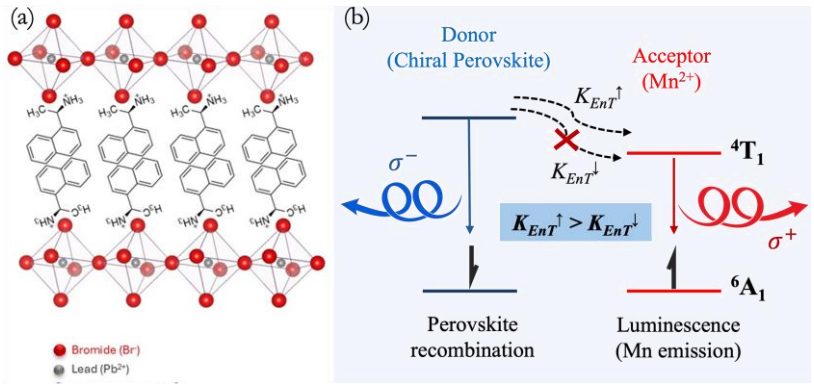
Highlights

Opposite-sign CPL from host and Mn emission in chiral 2D perovskites reveals spin-selective energy transfer enabled by spin–orbit coupling and dopant exchange interactions.

Resumo/Abstract

Circularly polarized luminescence (CPL) in chiral semiconductors provides a powerful platform for probing the interplay among structural chirality, spin–orbit coupling (SOC), and excited-state dynamics. In this work, we investigate CPL in a chiral 2D hybrid lead-bromide perovskite doped with Mn^{2+}, namely $(R/S\text{-NEA})_2PbBr_4$ (NEA = N-Ethylammonium), focusing on how Energy Transfer (EnT) from the perovskite host to localized Mn^{2+} emissive centers modulates the handedness and magnitude of the emitted CPL. Chiroptical measurements reveal opposite CPL signs associated with host excitonic emission and Mn-centered luminescence within the same enantiomeric material, indicating that chirality transfer is not governed solely by static structural effects. We explore the hypothesis that host-to-Mn EnT proceeds through spin-selective pathways enabled by SOC in the perovskite lattice and exchange interactions involving the Mn^{2+}dopant, as shown in the figure.

To rationalize these observations, we have developed cluster models that capture the local environment and symmetry-breaking features of the chiral perovskite lattice. TD-DFT calculations of absorption and circular dichroism spectra are employed to benchmark these models against experimental data. Preliminary results show excellent qualitative agreement with experiments, supporting the suitability of both the cluster models and the computational approach. In the next steps, we will compute electric and magnetic transition dipole moments, which enable the evaluation of rotatory strengths and provide microscopic insight into how local structure and dopant-induced interactions influence the magnitude and sign of the observed CPL. Together, these results elucidate the material's intrinsic electronic properties and clarify the roles of chirality and Mn doping in mediating spin-selective EnT, ultimately shaping the CPL response. This framework paves the way toward engineering CPL through excited-state spin control.



(a) The (NEA)2PbBr4 hybrid-perovskite. (b) Host-to-dopant spin-selective energy transfer mechanism.

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We would like to acknowledge the US Department of Energy and Prof. David Waldeck for collaborative discussions.

Photocatalytic Degradation of Methylene Blue Using Lanthanum-Modified Nb2O5

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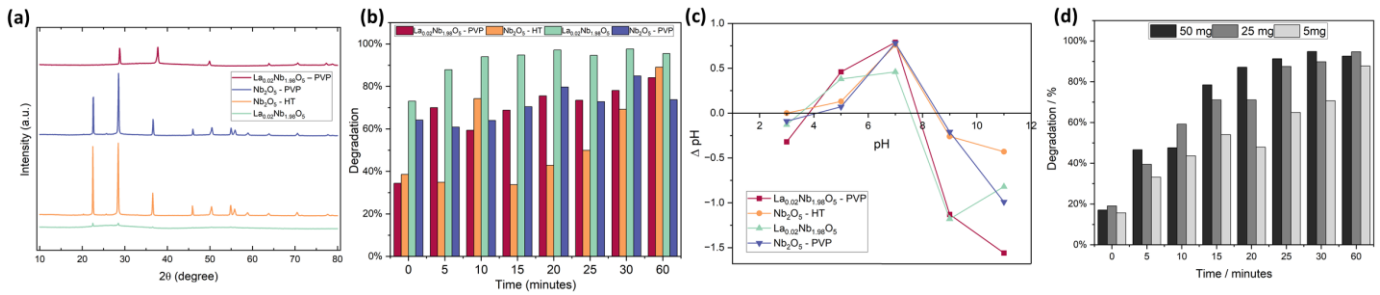
Palavras Chave:*Photocatalysis,Niobium pentoxide,Lanthanum,Methylene blue*

Highlights

La-modified Nb_2O_5 was synthesized hydrothermally. Lanthanum enhanced photocatalytic activity and reduced PZC. PVP addition impaired performance. Best degradation occurred under acidic conditions.

Resumo/Abstract

Industrial wastewater containing synthetic dyes represents a major environmental concern due to their persistence and resistance to conventional treatments. Photocatalysis using semiconductor materials has emerged as an effective strategy for dye degradation, among which niobium pentoxide (Nb2O5) has attracted attention due to its suitable bandgap, high chemical stability, and natural abundance. In this work, lanthanum-modified Nb2O5 catalysts were synthed hydrothermally (180 °C for 24 h) using lanthanum nitrate and commercial HY-340 Nb2O5 at a molar ratio of 0.02:1 (La:Nb). The influence of polyvinylpyrrolidone (PVP) as a stabilizing agent was also evaluated. The point of zero charge (PZC) of the catalysts was determined by the pH drift method. Photocatalytic performance was evaluated in a reactor at 30 °C containing 100 mL of a 5 ppm methylene blue (MB) solution at pH 4, 7, or 10 with 1 mL of 3% H2O2. Prior to irradiation, the suspension was stirred in the dark for 30 min to reach adsorption equilibrium, followed by UV irradiation (λ = 370 nm) for 1 h. Samples were centrifuged at 6000 rpm for 10 min and analyzed by UV-Vis spectrophotometry. Catalyst concentration was also investigated. After 1 h of irrradiation, Nb2O5-PVP showed the lowest activity, while La-modified Nb2O5 exhibited the highest photocatalytic performance. The enhanced activity is attributed to the presence of La species, which may act as electron traps, improving e-/h+ separation and facilitating the formation of reactive oxygen species in the presence of H2O2. In contrast, PVP addition may partially block active sites, which hinders photocatalytic performance. Catalysts containing La presented lower PZC values, indicating surface charge modifications that can influence dye adsorption. Although methylene blue is a cationic dye, the best photocatalytic performance was observed under acidic conditions, suggesting that radical generation and H2O2 activation play a dominant role in the degradation pro



a) XRD spectra; b) photodegradation efficiency; c) pH drift analysis & d) catalyst mass comparison.

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UFSC, CAPES, CNPQ, FAPESC, CACFM, GPM_3, LACFI, Nanoessência-UFSC, CBMM.

Photoleaching of chalcopyrite: influence of light wavelength on copper solubilization

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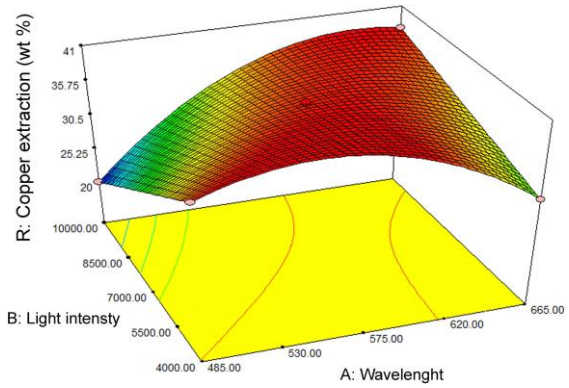
Palavras Chave:*Light; Semiconductor; Chalcopyrite; Leaching; Surface*

Highlights

Sustainable mining of critical minerals. Photocatalytic processing of copper ore. Enhancement of semiconductor solubilization kinetics under light irradiation.

Resumo/Abstract

Copper is an element extensively used in human activity. However, processing for the extraction of copper prevenient from chalcopyrite, the copper mineral most present on Earth's crust, is still done through pyrometallurgy. A viable option for pyrometallurgy is the (bio)hydrometallurgical methods, however, chalcopyrite is a refractory material with slow leaching kinetics. Several articles published recently point out that biohydrometallurgical processes combined with white light irradiation can increase the copper extraction rate from a chalcopyrite source, which is probably related to the fact that chalcopyrite is a semiconductor.
Using the electrochemistry of semiconductors approach as a starting point, this study investigated the effects of light on the chalcopyrite leaching in an acid solution containing ferrous or ferric ions. The effect of the radiation variables on the copper extraction rate was evaluated using the Response Surface Methodology (RSM), using a chemometric method.
Photoleaching experimental results show increased copper solubilization in an initial solution of 200 mmol L^{-1} Fe^{2+}, illuminated with high-intensity red, medium-intensity green, and low-intensity blue light. All illuminated experiments showed higher copper extraction in the acid solution containing 200 mmol L^{-1} Fe^{3+} than under the dark condition, emphasizing the effects of blue light at both high and low intensities. After photo-leaching experiments, X-ray diffraction analysis of the solid residue detected chalcopyrite, silicon dioxide, jarosite, and sulfur.
Cyclic voltammograms of chalcopyrite carbon paste electrodes under illuminated conditions showed an increase in current peaks and in the total electric charge passing through their surface.
These results indicate that the presence of illumination promotes copper extraction by leaching of chalcopyrite, and the radiation variables influence how light affects the chalcopyrite dissolution process.



Response surface for light-irradiated conditions initiated with only Fe^{2+}.

Agradecimentos/Acknowledgments

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Self-assembled drug delivery system functionalized with photoactive molecules

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Palavras Chave:*Drug delivery,Chitosan,Eosin Y,Nanoparticles,Photodynamic therapy*

Highlights

Photosensitive polymeric nanoparticles were obtained.

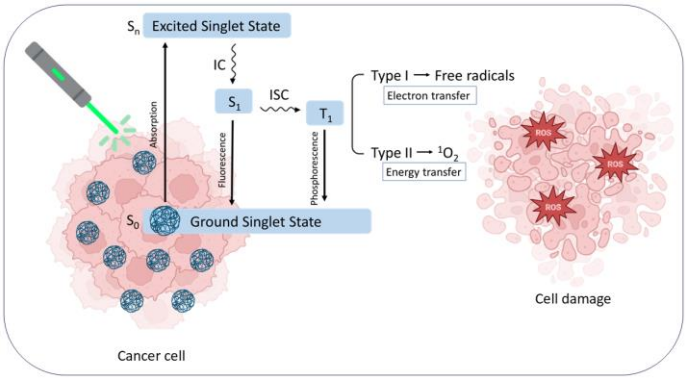
Nanoparticles exhibited efficient singlet oxygen generation.

The system demonstrated potential for application in photodynamic therapy.

Resumo/Abstract

The increasing incidence and mortality rates of cancer have intensified the search for minimally invasive therapeutic strategies. It is estimated that one in five individuals will develop the disease during their lifetime, with non-melanoma skin cancer being the most prevalent form. In this context, photodynamic therapy (PDT) emerges as a promising alternative, particularly through the development of nanosystems functionalized with photoactive molecules. These systems enable the selective delivery of photosensitizers to tumor cells, thereby enhancing therapeutic efficacy while minimizing damage to healthy tissues.

In this study, photosensitive polymeric systems were developed based on a cationic chitosan derivative, functionalized with the photosensitizer eosin Y (EY). ^{1}H NMR and FTIR spectroscopies confirmed the conjugation of the photosensitizer to HTCC, resulting in the HTCC–EY product. UV–Vis absorption and fluorescence emission analyses demonstrated that EY preserved its photoactive properties upon conjugation to the polymeric matrix. The incorporation of the nonionic surfactant F127 promoted the formation of self-assembled nanoscale structures (HTCC–EY/F127 NPs), as confirmed by dynamic light scattering (DLS), with particle sizes of approximately 200 nm and a zeta potential of around −25 mV. The singlet oxygen generation capability of the nanoparticles was evaluated through the photodegradation of uric acid under green light irradiation, monitored by the decrease in the absorption band at 290 nm. Kinetic profiles revealed efficient singlet oxygen production and demonstrated that EY conjugation to HTCC did not compromise its photodynamic activity. Furthermore, conjugation significantly reduced photosensitizer photobleaching, leading to enhanced photostability of the system. Overall, these findings indicate that the developed nanomaterial holds significant potential for PDT applications, particularly in the treatment of superficial cancers, such as skin cancer.



Schematic illustration of PDT application in cancer cells, highlighting ROS generation.

Agradecimentos/Acknowledgments

This work was supported by CNPq, CAPES, INCT-Catálise and INPIIF (Instituto Nacional de Pesquisa e Inovação em Imagem Fototérmica).

Spectroscopic study of naphthalimides aggregation in solution

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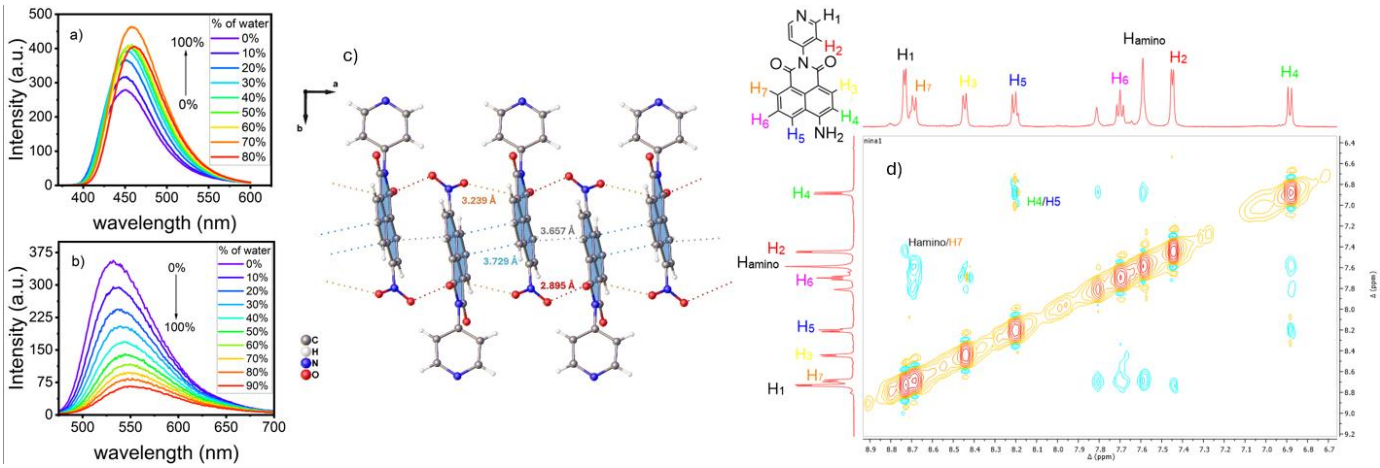
Palavras Chave:*aggregation, π-stacking, emission, NOESY*

Highlights

Aggregation of naphthalimides induces or quenches their luminescence. NOESY can be used to identify the formation of aggregates by detecting interaction through space.

Resumo/Abstract

1,8-Naphthalimides (NIs) are aromatic heterocycles widely known in the literature for forming aggregates through π-stacking, a type of intermolecular interaction between aromatic rings. When π-conjugated systems aggregate, they are susceptible to aggregation-induced emission or quenching, so that the possibility of either of these two phenomena occurring because of stacking is closely related to the molecular structure and packing modes. Understanding aggregation is essential to understand which effects will be observed. This study investigated the aggregation of 4-nitro-N-(pyridyl)-1,8-naphthalimide (NI-NO_2) and 4-amino-N-(pyridyl)-1,8-naphthalimide (NI-NH_2) in the solid state by X-ray structure determination and electronic spectroscopy in DMSO solutions, in which the molar fraction of water was varied. X-ray crystallography data for NI-NO_2 show the occurrence of aggregation assembled by p-stacking and hydrogen bonding (Figure 1). In solution, for the same concentration of NI-NO_2 (1.04×10^{-4} mol/L), an increase in emission intensity was observed with an increase in the proportion of water in solution, while for NI-NH2 (1.01×10^{-4} mol/L), the opposite effect was observed (Figure 1). Aggregation in solution was also evaluated by ^{1}H-NMR NOESY, but as a function of concentration rather than solvent variation. The result of the experiment is a two-dimensional spectrum in which the dipolar coupling between hydrogen interacting in space can be identified. The spectrum obtained for NI-NH_2 (1.82×10^{-2} mol/L) (Figure 1) showed evidence of stacking due to couplings unlikely to occur within the same molecule (Hamino/H7, H4/H5), indicating that this is an interaction between hydrogens from different molecules. In the next enrsteps of the work, the NOESY experiment of NI-NO_2 will be performed and new emission spectra will be recorded under different conditions to further study the aggregation of these NIs.



UV-visible emission of NI-NO2(a) NI-NH2(b) X-ray diffraction of NI-NO2(c) NOESY spectra of NI-NH_2(d)

Synthesis and Characterization of a Cationic Photosensitizer Derived from Rose Bengal B for Photodynamic Applications

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Palavras Chave:*Photodynamic Therapy,Synthesis of Photosensitizers,Xanthene,Rose Bengal B*

Highlights

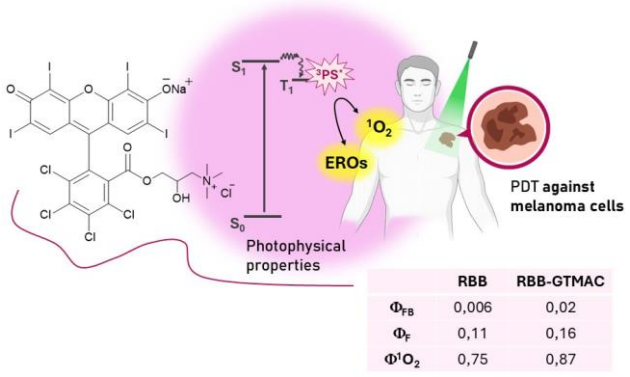
Cationic Rose Bengal B derivative has been synthesized;
Substituents group does not affect the photophysical properties of the PS;
The derivate showed photodynamic effects against melanoma cells.

Resumo/Abstract

The excitation of a photosensitizer (PS) by visible light, in the presence of molecular oxygen, leads to the formation of cytotoxic reactive oxygen species (ROs), which constitutes the fundamental principle of photodynamic therapy (PDT).[1] In the search for new PS, this work modified the structure of the PS Rose Bengal B (RBB) through the incorporation of the glycidyltrimethylammonium chloride (GTMAC) group, aiming to maintain a permanent positive charge in the molecular structure, thereby facilitating PS internalization and the dispersion of ROs within the intracellular environment. It was observed that the structural modification did not alter the spectroscopic profiles of RBB, although a significant decrease in the molar absorptivity coefficient was observed in polar environments, possibly associated with aggregate formation. The incorporation of the GTMAC group did not affect the hydrophilic/hydrophobic balance of the PS. Investigations of the photophysical and photodynamic properties of RBB-GTMAC revealed lower photostability of the derivative. The fluorescence quantum yield remained low. The ability to generate singlet oxygen ($^1O_2$) was confirmed using uric acid (UA) as a probe and a green laser (533 nm, 100 mW cm^{-2}), and first-order photodegradation kinetic models were identified. The results indicate that the functionalization did not alter the properties of the molecule, preserving the intrinsic and desirable characteristics of RBB. In*in vitro*biological assays against B16F10 cells, RBB-GTMAC was non-toxic up to a concentration of 1×10^{-4} mol L^{-1}. Under white light irradiation (55.3 J cm^{-2}), it was able to promote the inactivation of approximately 66% of melanoma cells in a single application. The synthesized RBB-GTMAC, preserved the physicochemical and photodynamic properties of RBB, demonstrating potential for future*in vivo*biological application studies and as a promising candidate drug for PDT.

Reference

[1]**Chem. Soc. Rev**., 2025, 54, 7749-7768



Scheme of the action of RBB-GTMAC in PDT and its photophysical properties

Agradecimentos/Acknowledgments

This work was supported by UFSC, CNPq, CAPES, INCT-Catálise and INPIIF.

Synthesis and photochemical investigation of an azo compound for Free Radical Polymerization under LED irradiation

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Palavras Chave:*Azo dyes,photopolimerization,LED,organic photocatalyst,organic photoinitiator*

Highlights

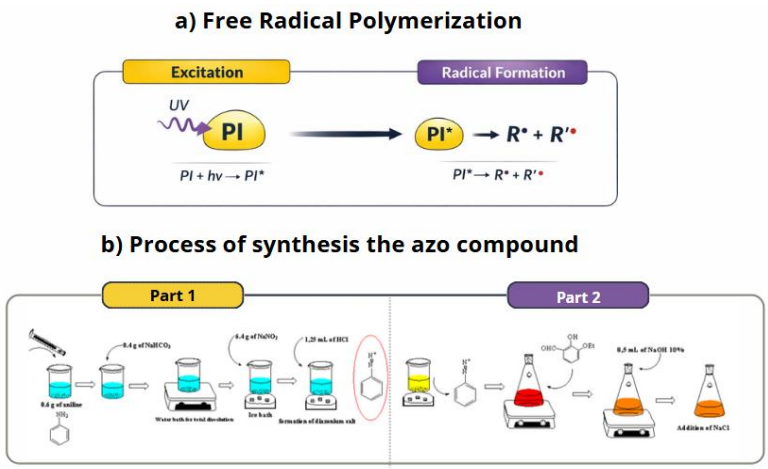
• The ethoxy-azo was synthesized and characterized by spectroscopic techniques.

• Ethoxy-azo was evaluated as a photoinitiator, achieving high monomer conversion under 365 nm LED irradiation.

Resumo/Abstract

Free Radical Photopolymerization (FRP) reactions are commonly described as a green technology due to their low electrical power and energy requirements, low-temperature operation, and absence of volatile organic compound release (solvent-free systems) [1]. Organic photoinitiator-based photoredox systems offer lower toxicity, compatibility with visible LEDs, and a more sustainable alternative to metal-based catalysts in photopolymerization [2] (Fig 1a). In this work, 3-ethoxy-5-phenyl-azo (ethoxy-azo) was synthesized in two steps. First, aniline reacts with HCl and $NaHCO_3$ to form the diazonium salt (solution 1). In the second step, the aldehyde is dissolved in NaOH (solution 2), which is then added to solution 1, promoting the coupling reaction and forming the azo dye. The ethoxy-azo was analyzed by the following spectroscopy techniques: UV-Vis, 1H NMR and was investigated as a photoinitiator in the FRP of ethoxylated trimethylolpropane triacrylate (TMPETA). Besides, FRP reaction was performed under laminate conditions using 1–3% photoinitiator (0.5 g TMPETA) and LED irradiation at 365 nm. Monomer conversion was monitored by FTIR at 1636 cm^{-1}. The ethoxy-azo showed efficient performance in all systems, with optimal results at 3%, reaching 80% conversion due to enhanced radical generation. Lower concentrations resulted in slower kinetics and reduced conversion.

BONARDI, A.-H. et al. Organometallic vs organic photoredox catalysts for photocuring reactions in the visible region.**Beilstein Journal of Organic Chemistry**, v. 14, p. 3025–3046, 12 dez. 2018. LALEVÉE, J.; TEHFE, M.-A.; MORLET-SAVARY, F.; GRAFF, B.; DUMUR, F.; GIGMES, D.; BLANCHARD, N.; FOUASSIER, J. P. Photoredox catalysis for polymerization reactions.*Chimia*, v. 66, n. 6, p. 439–441, 2012.



Ilustration of the FRP reation and the process of the synthesis of the fotoinitiator (azo compound)

Agradecimentos/Acknowledgments

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Synthesis, characterization, and photophysical properties of a fluorescent coumarin

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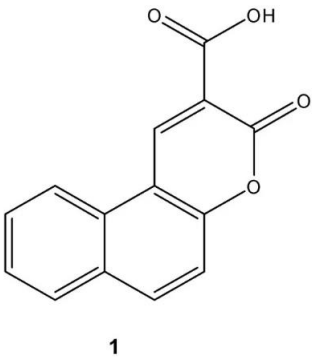
Palavras Chave:*coumarin,fluorescent optical devices,polymeric films,functional materials*

Highlights

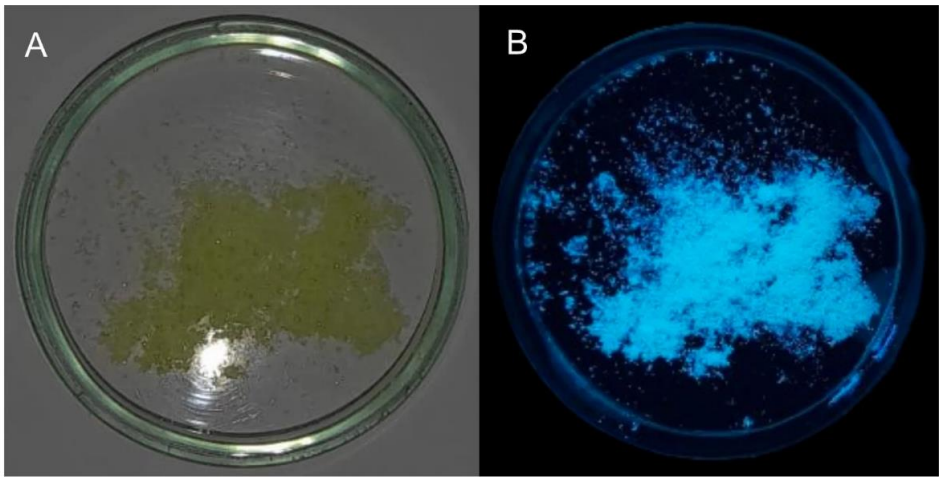
Coumarin derivative synthesized with 51% yield.Structure confirmed by IR, NMR, and single-crystal X-ray diffraction.Blue emission in solvents and embedded in PMMA film.

Resumo/Abstract

Coumarins represent an important class of natural fluorophores, found for instance in tonka bean seeds (Dipteryx odorata), and are distinguished by their internal charge transfer properties and broad applicability as fluorescent probes. In this work, coumarin derivative**1**(5-((2-hydroxynaphthalen-1-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione;**Figure 1**), was synthesized via the condensation of 2-hydroxy-1-naphthaldehyde with Meldrum's acid, using pyrrolidine as a base. The product was obtained as a crystalline yellow solid in 51% yield, and its structure was confirmed by infrared spectroscopy, ^{1}H and ^{13}C NMR, and single-crystal X-ray diffraction. The spectroscopic behavior of the compound was examined in various organic solvents using UV-vis and fluorescence techniques, revealing blue emission under UV excitation and intensity variations associated with solute–solvent interactions. Additionally, the coumarin was incorporated into a polymethyl methacrylate (PMMA) matrix, producing a fluorescent film that preserved its photophysical properties in the solid state. These findings highlight the potential of the synthesized coumarin as a fluorescent material in both solution and polymer films, contributing to the development of luminescent systems with applications in functional materials and photophysical studies.



1



Structure of coumarin 1 and samples of the compound exposed to (A) natural and (B) UV light.

Agradecimentos/Acknowledgments

CNPq (Process numbers 407774/2021–1 and 311387/2023-3), Instituto Nacional de Pesquisa e Inovação em Imagem Fototérmica (INPIIF/CNPq; process number 408454/2024-5), CAPES (Finance code 001), and FAPESC (Process number: 2024TR002301).

Theoretical Photochemistry of Amazonian Xanthones: A QTAIM and TD-DFT Study with Implications for ESIPT

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Palavras Chave:*Amazonian Xanthones, ESIPT, TD-DFT, QTAIM, Photochemistry.*

Highlights

We demonstrate that S1 electronic redistribution, rather than ground-state preorganization, dictates a barrierless proton transfer in Amazonian xanthones.

Resumo/Abstract

We investigate the aqueous-phase photochemistry of five newly discovered Amazonian xanthones (XAN1–5) [1,2] using DFT and TD-DFT (B3LYP-D3(BJ) and CAM-B3LYP) combined with QTAIM and VDD analyses. Ground-state results show that all derivatives form stable intramolecular O–H···O Hbonds (-10.3 to -11.8 kcal/mol) with significant charge polarization. However, excited-state intramolecular proton transfer (ESIPT) is selectively observed only for XAN2, XAN3, and XAN4. Minimum Energy Path (MEP) calculations reveal that while ground-state preorganization is essential, it is not a sufficient predictor of ESIPT. Instead, the process is governed by specific electronic redistribution in the S_1 state, which enhances acceptor basicity and leads to a nearly barrierless proton transfer with stabilization energies of 13.6–14.4 kcal/mol. This mechanism results in remarkably large Stokes shifts (>217 nm), providing a dual-region spectroscopic fingerprint (UV-absorption/visible-emission). Our findings elucidate the photochemistry of these natural chromophores and offer a guide for designing new photoactive antioxidant compounds and molecular probes.

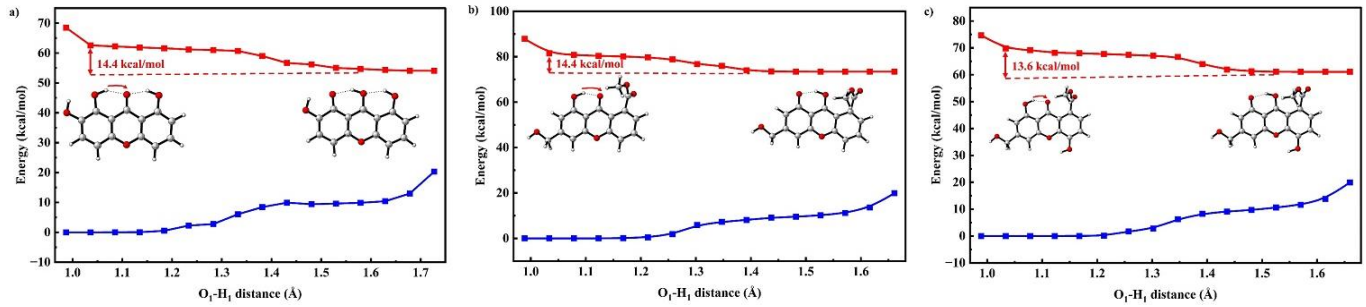


Figure 1. B3LYP-D3(BJ)/def2-TZVPP Minimum Energy Paths (MEP) for S0 (in blue) and S1 (in red) states

Agradecimentos/Acknowledgments

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2D Triangular Coordination Networks: Zero-Field Single-Ion Magnet Behavior in the Co(II) System with a Negative Anisotropy

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Palavras Chave:*Coordination networks,Magnetic easy-axis anisotropy,Single-ion magnets*

Highlights

First M(II)–dps coordination networks with an oxamate derivative yielding isolated single-ion units. The dps ligand forms in situ from dpds. Zero-field SIM with easy-axis anisotropy in Co(II) nodes.

Resumo/Abstract

In the early 2000s, the observation of slow magnetic relaxation in mononuclear rare-earth double-decker systems marked a pivotal moment in the development of molecular nanomagnetism,[1] giving rise to single-ion magnets (SIMs). A decade later, in 2010, the first SIM based on a mononuclear trigonal-pyramidal Fe(II) complex was reported, highlighting the growing potential of first-row transition metals in this field.[2] With these considerations in mind, we employed the node-and-spacer approach as the central synthetic design strategy. Two coordination networks from Co(II) and Cu(II) nodes: $[\{Co(H_2mpba)(dps)\}\cdot 2DMSO]_n$**(1)**and $[\{Cu(H_2mpba)(dps)\}\cdot 2DMSO\cdot H_2O]_n$**(2)**[$H_4$mpba = 1,3-phenylenebis(oxamic) acid and dps = 4,4′-dipyridyl sulfide]were isolated via a diffusion method under ambient conditions and fully characterized in the solid state, including magnetic measurements and*ab initio*theoretical calculations.[3] Interestingly, the starting 4,4′-dipyridyl disulfide (dpds) ligand underwent*in situ*transformation into dps at room temperature, yielding isomorphic two-dimensional triangular coordination networks. In each triangular motif, two metal centers are bridged by dps ligand, while the third is linked by H_2mpba^{2-} ligand, resulting in well-isolated M(II) ions. Magnetic measurements revealed that compound**1**exhibits zero-field single-ion magnet behavior with slow magnetic relaxation.*Ab initio*calculations yielded a large negative axial zero-field splitting parameter (D = −106.0 cm^{-1}), in close agreement with the experimental value (D = −103.7(7) cm^{-1}), confirming strong easy-axis magnetic anisotropy. In contrast, compound**2**shows a bottleneck effect under an applied magnetic field of 1 kOe (n = 2.0(1)), indicative of field-induced slow magnetic relaxation.

[1] N. Ishikawa*et al*.,*J. Am. Chem. Soc.*, 2003, 125 (29), 8694.

[2] W. H. Harman*et al*.,*J. Am. Chem. Soc.*, 2010, 132(51), 18115.

[3] L.D.G. Botelho et al.,*RSC Advances*, 2026, 16, 2179.

Agradecimentos/Acknowledgments

FAPEMIG (APQ-00544-23, APQ-05218-23, master's fellowship), FAPERJ, and NACAD for supporting this work. M.V.M. gratefully acknowledges FAPEMIG and CNPq Foundations, Brazil, through a research productivity fellowship (BPQ-APQ06579-24).

Accurate thermal sensing via upconversion luminescence thermometry enabled by denoising neural networks

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Palavras Chave:*Rare-earths,Optical materials,Thermometers,Machine Learning,Accurate thermal sensing*

Highlights

A constrained signal-to-noise ratio increases the uncertainty of luminescent thermometers.

U-Net denoising algorithm enables accurate luminescence thermometry in harsh conditions.

Resumo/Abstract

Accurate and remote temperature sensing at the sub-micron and nanoscale is critical for applications ranging from monitoring intracellular dynamics to managing heat in microelectronic devices[1]. Luminescent thermometers are well-suited for these tasks; however, their practical deployment is often constrained by environmental cross-sensitivity that can mimic temperature-induced spectral changes[1]. In biological media, in particular, weak emission signals due to low excitation power and light-tissue interactions degrade thermal resolution by increasing temperature uncertainty (δT)[1]. To address this limitation, we integrate convolutional neural networks (CNNs), using a U-Net method, to reconstruct temperature-dependent emission spectra from low signal-to-noise ratio (SNR) measurements. As a proof-of-concept, a bixbyite-type La_2O_3:Yb^{3+}(10 at.%),Er^{3+}(1 at.%) phosphor was synthesized via solid-state reaction, and temperature-dependent upconversion spectra (980 nm Yb^{3+} excitation) were acquired from 223 to 323 K under excitation powers of 50, 100, and 500 mW (assays**A**,**B,**and**C**, respectively). By employing the $^2H_{11/2}$/$^4S_{3/2}$intensity ratio as the thermometric parameter, the thermometer' calibration yielded relative sensitivities (Sr) near 1.3% K^{-1} at 320 K across all power regimes. Despite this comparable sensitivity, δT at 320 K was strongly SNR-dependent, reaching 1.2 K for assay**A**, being 4.3-fold higher than that for assay**C**(0.28 K). After U-Net denoising, δT decreased to 0.49 K for assay**A**, corresponding to an improvement of ≈41% relative to the raw spectra. To assess robustness, the same model was applied to assay**B**, resulting in a 28% reduction in δT (from 0.76 K to 0.55 K), thereby demonstrating reproducible performance gains. Collectively, these results highlight how advanced data-driven approaches can enable accurate thermometric readouts even under signal-limited conditions, stepping further into potential applications.

[1] L. Ming,*et al.*,*Adv. Mater.*2023, 35, 52.

Agradecimentos/Acknowledgments

FAPESP 2023/05718-9; CAPES 88887.686388/2022-00; CNPq 309448-2021-2, 308868/2022-6, 305313/2024-0; Laboratory of Functional Materiais – IQ Unicamp.

Addressing ligand affinities of isoquinolines in triruthenium acetates using tandem mass spectrometry

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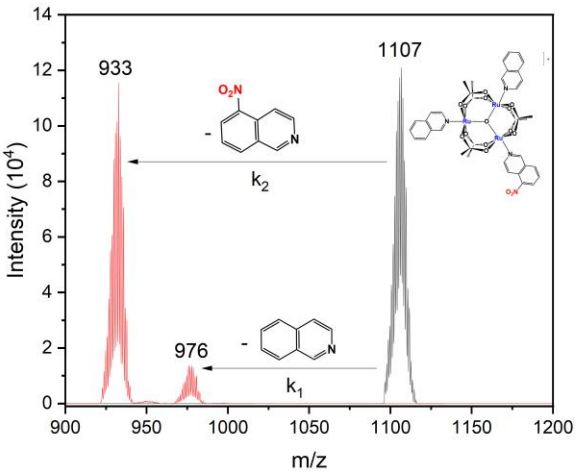
Palavras Chave:*trirtuhenium acetates,isoquinoline,mass spectrometry,triruthenium acetates,isoquinoline,mass spectrometry*

Highlights

Using collision-induced dissociation experiments, we have found that the ligand affinity of isoquinolines in triruthenium acetates relates to the ligand's σ-donor character.

Resumo/Abstract

The chemistry of triruthenium acetates has been explored for catalytic applications, electron-transfer processes, biological activity, and extended structures. The ancillary ligands in these complexes are important for modulating their chemical properties for the desired application. In this way, triruthenium clusters bearing azonaphtalene ligands were reported as potential anticancer and antitrypanosomal agents and as a promising nitric oxide donor (*Coord. Chem. Rev. 494, 2023)*. Even though N-heterocycles are inert ligands in triruthenium complexes, we have recently found the spontaneous dissociation of isoquinoline as a side reaction of the orthometallation of phenanthrolines. Thus, understanding the affinity of the ancillary ligand to the metal can be a useful tool for planning reactions in the future. Using collision-induced dissociation experiments, we have explored the relative ligand affinity of substituted isoquinolines for the complex $[Ru_3O(CH_3COO)_6(iq)_2(L)]PF_6$, where iq = isoquinoline and L = 5-nitroisoquinoline ($iqNO_2$), 5-bromoisoquinoline (iqBr), pyridine (py), 5-methoxyisoquinoline ($iqOCH_3$), and 5-aminoisoquinoline ($iqNH_2$). The dissociation in the parent ion $[Ru_3O(CH_3COO)_6(iq)_2L]^+$ has two competitive paths by the dissociation of iq or L. In fact, the CID of all five complexes leads to both dissociations in different ratios, which can be related to the ligand affinity by the Cooks' method. By this analysis, we found the affinities of L with respect to isoquinoline: $iqNO_2$ < iqBr < py < $iqNH_2$ < $iqOCH_3$. As found for pyridine analogue complexes, the affinity trend corresponds to the electronic character of the ligand, in a way that stronger σ- or Π-donor ligands give higher affinities. The inconsistency of the amino and methoxy substituents might be attributed to the possibility of the first ligand coordinating by the amino group rather than the nitrogen in the aromatic ring.



CID of [Ru3O(CH3COO)6(iq)2(iqNO2)]+ (m/z = 1107) at 0 (black) and 30 NCE (red).

Agradecimentos/Acknowledgments

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Ag(I) complexes containing thiosemicarbazone and 1,10-phenanthroline derivatives: synthesis, characterization and antibacterial activity investigation

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Palavras Chave:*Silver Complexes,Antibacterial Activity,Synthesis,1,10-phenanthroline*

Highlights

Ag(I) complexes with TSC and Phen were synthesized and characterized by ^{1}H NMR, FTIR and UV-Vis. Antibacterial activity evaluation highlights the action of the complexes against microbial resistance.

Resumo/Abstract

The growing bacterial resistance to conventional pharmaceuticals is a global public health challenge, demanding the development of new bioactive compounds. Silver(I) complexes have attracted great interest in medicinal chemistry due to their intrinsic antibacterial properties, low toxicity to human cells at controlled concentrations, and remarkable chemical stability. This work describes the synthesis and characterization of new Ag(I) complexes coordinated to two classes of ligands: thiosemicarbazone derivatives (TSC) and 1,10-phenanthroline derivatives (Phen), resulting in compounds with the general formula [Ag(TSC)(Phen)]. The investigation sought to understand the synergistic influence of these ligands when simultaneously coordinated to the metallic center. The synthesis was conducted in two steps: obtaining the ligands followed by the formation of the metallic complexes. Characterization by UV-Vis spectroscopy revealed a significant bathochromic shift in the TSC bands, providing clear evidence of coordination to the Ag(I) ion. FTIR spectra confirmed the coordination through changes in the stretching frequencies of the C=N and C=S groups. In the ^{1}H NMR analysis, the signals of the aromatic protons from the TSC phenyl ring (in the 6-8 ppm region) showed chemical shifts and changes in the multiplicity pattern, phenomena attributed to the electronic density redistribution induced by the metal-ligand bond. Molar conductance measurements in organic solvents indicated values compatible with 1:1 electrolytes, suggesting a structure composed of a complex metallic cation and a free nitrate counterion (NO_3^-). After structural elucidation, the biological potential of the compounds was evaluated through antibacterial activity assays, aiming to verify the action potential against different microorganisms.

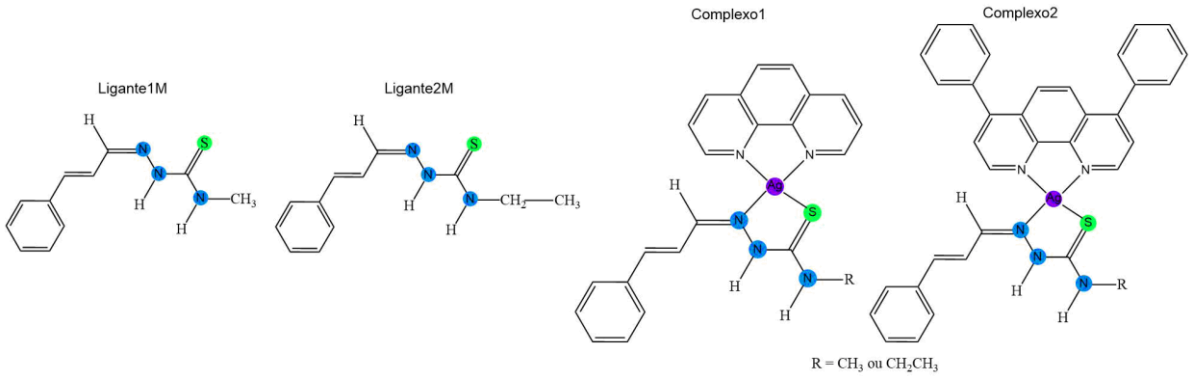


Figure 1: Structure of the synthesized and characterized molecules.

Agradecimentos/Acknowledgments

Thanks to CAPES, CNPq (305259/2025-3), and FAPESP. Special thanks to CCQM colleagues for their fundamental collaboration and to my friends for all the support and encouragement.

Análises condutimétrica e espectroscópica vibracional de eletrólitos de interesse para baterias de Mg(II) e híbridas contendo Mg(II)/Li(I)

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Palavras Chave:*Baterias de magnésio,eletrólitos,condutividade iônica,espectroscopia Raman,estruturas de solvatação.*

Highlights

Two $Mg(CF_3SO_3)_2$-based systems show conductivities comparable to Li(I) technology and the Raman spectra evidence the lack of neutral Mg(II) aggregates, which do not contribute to the charge transport.

Resumo/Abstract

Embora o metal Mg seja mais abundante, tenha maior capacidade volumétrica quando comparada ao metal Li (Mg = 3833 mAh/mL; Li = 2062 mAh/mL) e maior segurança operacional devido à baixa tendência de formação de dendritos, a comercialização de baterias recarregáveis de magnésio (BRM) é ainda limitada principalmente pela incompatibilidade dos eletrólitos com os materiais cristalinos comumente utilizados na fabricação do catodo, cujas as fortes interações eletrostáticas com o cátion Mg(II), de alta densidade de carga, diminuem substancialmente a cinética de inserção e desinserção. Neste contexto, eletrólitos híbridos de Mg(II)/Li(I) têm surgido como boas opções, pois combinam a seguridade do ânodo de Mg com a cinética de inserção/desinserção mais rápida de Li(I). No presente trabalho, dois novos eletrólitos à base de $Mg(CF_3SO_3)_2$ e híbridos contendo LiCl, em uma mistura equimolar de tetraidrofurano (THF) e*N*,*N*-dimetilformamida (DMF), são estudados. Ambos sistemas exibem condutividades iônicas superiores a 9 mS cm^{-1}, cujo o comportamento é muito bem explicado pelos espectros Raman. O modo vibracional mais sensível de $CF_3SO_3^-$, $\delta_s(CF_3)$, revela somente a presença de uma banda muito intensa em 754 cm^{-1} e uma outra de menor intensidade em 758 cm^{-1}. A primeira é relacionada ao ânion não coordenado e a segunda corresponde a pares iônicos de contato (PIC) do tipo 1:1, $Mg^{2+}..CF_3SO_3^-$ e $Li^+..CF_3SO_3^-$. De fato, a última banda é mais intensa no eletrólito híbrido devido à contribuição de ambos arranjos, mas as condutividades iônicas são ligeiramente menores em virtude da carga global nula do PIC à base de Li. As bandas mais sensíveis de THF e DMF mostram a participação de ambos solventes na esfera de coordenação dos cátions e efeito preferencial da amida. Este trabalho abre portas para futuros testes de compatibilidade não somente com catodos cristalinos, mas também com materiais orgânicos, onde a difusão do cátion de metal alcalino terroso é facilitada pelas interações mais fracas.

Agradecimentos/Acknowledgments

Agradeço ao Departamento de Química da Universidade Federal de Juiz de Fora e ao programa de Pós-graduação em Química pelo apoio à pesquisa desenvolvida. Às agencias de fomento Capes e Fapemig pelo apoio financeiro ao trabalho realizado.

A novel antimicrobial copper trans-cinnamate prototype against the resistance phenomenon.

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Palavras Chave:*antibacterial activity,trans-cinnamic acid,copper sulfate,antimicrobial resistance*

Highlights

A novel copper complex against antimicrobial resistance; Prototype synthesized using trans-cinnamic acid and copper sulfate; Antimicrobial assays demonstrate activity against pathogens.

Resumo/Abstract

Antimicrobial resistance occurs when microorganisms undergo genotypic and metabolic changes. The exposure to selective pressure agents results in the loss of drug efficacy to antimicrobial agents, with an increasing of the risk of dissemination and pathogenicity. In this scenario, the development of new prototypes in bioinorganic chemistry becomes essential. Materials capable of exhibiting greater therapeutic efficiency and reduced deactivation by bacterial resistance mechanisms, potentially representing the only alternative in specific cases. In this context, the World Health Organization (WHO) classifies antimicrobial resistance as one of the top ten global health threats. This study aimed to synthesize and characterize a new copper complex with potential antimicrobial activity using trans-cinnamic acid as a ligand. As a strategy, the deprotonated form of the ligand may stabilize the metal and optimize its biodistribution. The complex was obtained with copper sulfate and trans-cinnamic acid in a 1:2 molar ratio, in a basic medium, over 40 minutes at room temperature, using a protic solvent. The structure of the complex was confirmed through spectroscopic techniques and thermogravimetric analysis, corresponding to ML_2, with L_2 referring to two coordinated trans-cinnamic acid ligands. Antibacterial assays demonstrated activity against*Staphylococcus aureus*and*Escherichia coli*, with a value of 34 µg L^{-1}, compared to the positive control (silver sulfadiazine). These results highlight the high potential of the copper complex as a prototype antimicrobial agent.

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A Red-Emissive Ir(III) Complex for BSA Detection and Quantification: Synthesis andCharacterization

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Palavras Chave:*Ir(III) complex,Protein sensing,Red emission*

Highlights

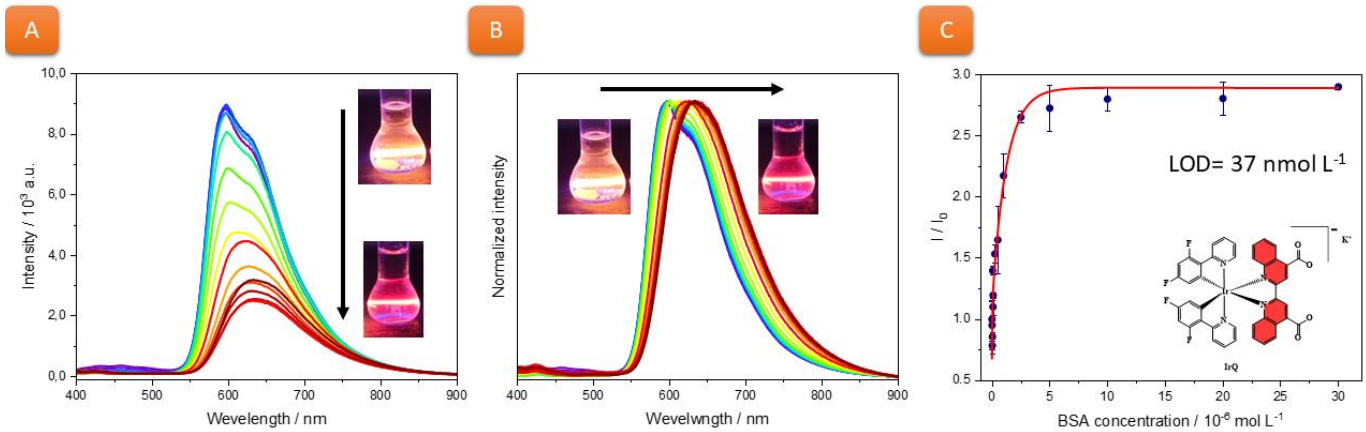
Detection and quantification of BSA protein by a red-emitting Ir(III) complex

Resumo/Abstract

Luminescent Ir^{3+} complexes are widely used in applications like sensing of biological and inorganic molecules. Their emission properties are related to strong spin–orbit coupling, which allows relaxation of the spin selection rule by generating a hybrid low-energy emissive state, ^{3}LC–^{1},^{3}MLCT.[1] Due to the influence of the environment on their excited states, they can be employed for the identification and quantification of proteins, such as bovine serum albumin (BSA).[2] BSA plays a critical role in the diagnosis and treatment of diseases such as liver cirrhosis. An Ir^{3+} complex, $K[Ir(Fppy)_2(bqdc)]$, was synthesized, Fppy = 2-(2,4-difluorophenyl)pyridine, bqdc = 2,2′-biquinoline-4,4′-dicarboxylate. This complex was characterized by FTIR, elemental analysis, HRMS, ESI-TOF, NMR, UV–vis, and PL. To evaluate it as a BSA sensor, solutions with and without protein were prepared while varying the complex concentration in the presence of BR buffer at pH 2.5. An optimal complex concentration of 10^{-5} mol L^{-1} was selected and used in the detection limit experiments, in which the protein concentration was varied. A shift in the emission maximum was observed, ranging from 590 nm at higher BSA concentrations to ~ 635 nm in the absence of protein. Additionally, a change in the emission profile was detected, transitioning from a more vibronic profile, characteristic of a predominantly ^{3}LC emissive state, to a Gaussian profile, characteristic of a predominantly ^{3}MLCT state. Emission intensity was the parameter most affected by the presence of the protein, being almost completely suppressed in its absence.. Therefore, emission intensity was selected as the analytical parameter for determining the limit of detection to be 37 nmol L^{-1}. These results demonstrate that the complex $K[Ir(Fppy)_2(bqdc)]$ is a valid sensor for the identification and quantification of BSA protein.

[1]SILVA, Renan C. et al.**Dalton Transactions**, 2024.

[2]HUANG, Chao et al.**Dalton Transactions**, 2018.



A: emission spectra of Ir(III) complex with protein; B: emission spectra normalized; C: LOD.

Agradecimentos/Acknowledgments

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A Scintillator-Photosensitizer Nanoplatform for X-Ray-Induced Photodynamic Therapy via Combined ROS Generation and Nitric Oxide Release

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Palavras Chave:*X-ray-induced photodynamic therapy (X-PDT),Perovskite CsPbBr3,Ruthenium(II) Complex,Reactive Oxygen Species (ROS),Nitric Oxide Release*

Highlights

Dual-action X-PDT nanoplatform integrating perovskite and NO-donor ruthenium(II) complex.

X-ray activation triggers ROS generation and NO release.

Resumo/Abstract

Despite advances in oncology, conventional treatments such as surgery, chemotherapy, and radiotherapy (RT) still present significant limitations, including severe side effects, tumor heterogeneity, and therapeutic resistance. In this context, X-ray-induced photodynamic therapy (X-PDT), which combines RT and PDT through scintillating nanomaterials capable of activating photosensitizers in deep tissues, has emerged as a promising alternative. In this work, we propose a dual-action X-PDT strategy integrating scintillators with ruthenium(II)-based photosensitizers, enabling simultaneous ROS generation and nitric oxide (NO) release, inducing synergistic oxidative and nitrosative stress to enhance cancer cell death. Among the different nanomaterials, the perovskite $CsPbBr_3$ stands out due to its intense radioemission at 515 nm. In this work, $CsPbBr_3$ was synthesized*in situ*within mesoporous silica, followed by pore sealing to improve biocompatibility and preserve its luminescent properties in aqueous media[1]. The nanoparticle was functionalized with 3-(aminopropyl)triethoxysilane (APTES) and covalently conjugated to a nitric oxide (NO)-donor ruthenium(II) complex ($RuNO_2$) via EDC/NHS coupling. X-ray diffraction of SiO_2@$CsPbBr_3$ confirmed the formation of the cubic $CsPbBr_3$ phase. Transmission electron microscopy showed spherical silica particles containing $CsPbBr_3$ distributed within their interior. The zeta potential changed from −20.1 to +25.5 mV after APTES functionalization, confirming the introduction of amine groups onto the nanoparticle surface. Singlet Oxygen Sensor Green (SOSG) assays demonstrated that SiO_2@$CsPbBr_3$ generates singlet oxygen ($^1O_2$) under X-ray irradiation. Chronoamperometric experiments using a selective NO sensor showed that the conjugated system SiO_2−NH_2−$RuNO_2$@$CsPbBr_3$ releases NO under ionizing radiation, highlighting its potential as a nanoplatform for X-ray-activated cancer therapy.

[1] Carulli, F. et al., S. ACS Energy Lett. 2023.

Agradecimentos/Acknowledgments

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Bio-Assisted Synthesis of Co3O4 from Marine Macroalgae Ethanolic Extract toward Efficient Oxygen Evolution Electrocatalysis

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Palavras Chave:*OER,Cobalt oxide,Renewable energy,Green synthesis*

Highlights

* Bio-assisted synthesis of spinel Co_3O_4 using *Sargassum* sp. extract
* Sustainable macroalgae valorization for OER electrocatalysis
* 382 mV overpotential at 10 mA cm^{-2} in 1.0 M KOH

Resumo/Abstract

Although electrolytic hydrogen (H_2) production is a promising route toward clean energy, it still faces significant challenges, particularly the high cost of catalysts required to efficiently drive water electrolysis. To address this limitation and contribute to the development of more sustainable and economically viable strategies for green hydrogen production, recent studies have explored biosynthetic routes for the preparation of efficient nanomaterials as electrocatalysts for the Oxygen Evolution Reaction (OER) [1]. In this context, a Co_3O_4 structure was synthesized using an ethanolic extract of the macroalgae *Sargassum sp*. as a bio-based precursor. Fourier-transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD) analyses confirmed the formation of the spinel cubic crystalline phase and the expected chemical composition of the material. The as-prepared Co_3O_4 exhibited excellent electrocatalytic performance in alkaline aqueous medium (1.0 M KOH), achieving an overpotential of 382 mV at a current density of 10 mA cm^{-2}. These electrocatalysts exhibited activity comparable to those reported in the literature [2]. Thus, this work provides a sustainable pathway for the valorization of abundant marine macroalgae biomass along coastal regions, enabling the production of high value-added materials that contribute to the advancement of clean and renewable energy technologies.

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[2] Raimundo RA, et al. Green synthesis of Co3O4 nanoparticles using psyllium husk (Plantago Ovata) and application as electrocatalyst for oxygen evolution reaction. Journal of Electroanalytical Chemistry 2023;932:117218. https://doi.org/10.1016/j.jelechem.2023.117218.

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Brushite (CaHPO4.2H2O) from industrial waste and its potential as a slow-release phosphate fertilizer

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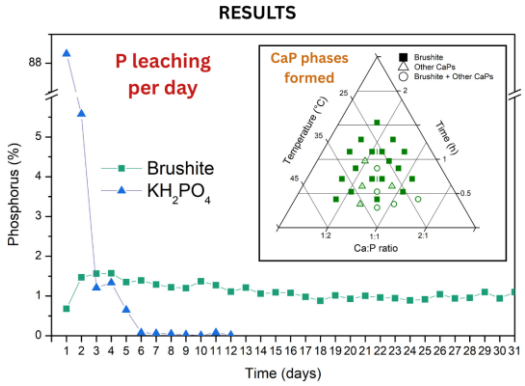
Palavras Chave:*brushite,phosphate,fertilizer,waste*

Highlights

This work presents the use of waste containing calcium ions to synthesize brushite, study its reaction conditions and the material's potential as a slow-release fertilizer.

Resumo/Abstract

Phosphorus is an essential macronutrient for the plant's growth, and Brazil is one of the main consumers of phosphate fertilizers due to the high agricultural production. Even though there are well-established phosphate fertilizers on the market, their inefficiency induces the need to develop improved fertilizers able to supply plants´ demand rate for nutrients. A slow-release fertilizer is the key to avoid the application of high concentrations of nutrients at once, and some inorganic solids containing phosphate are showing promising results as alternative fertilizers. Dicalcium phosphate dihydrate (DCPD), or brushite, is a calcium phosphate with the formula $CaHPO_4.2H_2O$ that has Ca/P molar ratio of 1, and interlayer water molecules, which conveys interesting properties for agricultural applications, especially regarding its solubility, allowing slow release of the phosphorus caused by the partial dissolution of the solid with water.[1] In this work, brushite was synthesized in a precipitation reaction with a buffer solution at pH 6.8 as the phosphate source, and an industrial residue as the source of calcium, obtained from another synthesis' supernatant. This synthesis uses remaining calcium in the mother liquor from hydrocalumite synthesis, which configures a sustainable process. Various reaction conditions were studied, including Ca:P molar ratio (1:2, 1:1 and 2:1), temperature (25, 35 and 45 °C) and reaction time (0.5, 1 and 2 h), and the phases formed were determined by powder X-ray diffraction (XRD) analysis. It was observed that brushite tends to rapidly form in Ca:P of 1:2 at room temperature, however it dehydrates to convert to monetite ($CaHPO_4$), as determined by periodic XRD analysis (Fig. 1). Finally, the phosphorus leaching rate was quantified with a fixed column method, to evaluate brushite's potential to slowly release the phosphate.
[1]Coker*et al.*Journal of Soil Science and Plant Nutrition 25, 2085-2097 (2025).



Ternary diagram of phases formed in all synthesis and phosphorus leaching percentage per day.

Agradecimentos/Acknowledgments

The author thanks CNPq and Conatus Ambiental for financing this work, and LIFQ (RRID:SCR_027389) from CEMUIQ-UNICAMP for technical support.

Can we get there? Pitfalls and Optimization of the Multi-Step Synthesis of Dinuclear Co and Cu Oxamate-based Complexes

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Palavras Chave:*Dinuclear Complexes,Oxamate,Precursors*

Highlights

This work aims the optimization of a multi-step synthesis and characterization of dinuclear oxamate-based complexes containing Co(II) or Cu(II) ions from*o*-phenylenediamine as the starting point.

Resumo/Abstract

The study of coordination compounds that vary in structure, ligands, and nuclearity offers vast possibilities and is of great interest to the design of advanced molecular materials. By that standpoint, this project is focused on the synthesis and study of the magnetic and redox properties of complexes based on the N,N',N'',N'''-1,2,4,5-benzenetetrailtetrakis(oxamate) (btto) ligand, and Co(II) or Cu(II) ions. As starting compound, we used 1,2-phenylenediamine, then subjected it to a multi-step synthetic route. On the first step (synthesis of*N*,*N*′-ditosyl-1,2-phenylenediamine), after several tries, due to obtaining mixtures that were difficult to separate (probably mono- and ditosylated product), we used an alternative route, by increasing the temperature (from 60 to 100 °C), using excess tosyl chloride, and avoiding the use of HCl. Accordingly, the reaction time was substantially reduced from 12 hours to 1.5 hours. NMR ^{1}H (DMSO-d_6, 500 MHz) showed chemical shifts consistent with the expected product (ppm): 2.35 (s, 6H); 6.99 (m, 4H); 7.35 (d, 4H); 7.59 (d, 4H); 9.28 (s, 2H). On the second step, the nitration of*N*,*N*′-ditosyl-1,2-phenylenediamine was carried out. NMR ^{1}H (DMSO-d_6, 500 MHz) showed chemical shifts consistent with the expected product (ppm): 2.38 (s, 6H); 7.38 (d, 4H); 7.70 (d, 4H); 7.79 (s, 2H). The samples were also characterized by IR spectroscopy and melting point measurements. The following phase will involve the preparation of the oxamate-based complexes, optimization of the crystallization processes, and investigation of their magnetic and redox properties. Interesting results are expected to be found due to the potential of such compounds of forming extended structures of higher nuclearity because of the free coordination sites in the oxamate units, and the ability of oxamate derivatives with aromatic spacers to mediate magnetic interactions and influence electronic properties.

Agradecimentos/Acknowledgments

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Caracterização de novos compostos de coordenação a partir da quitosana e salicilaldeído com zinco, manganês e níquel

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Palavras Chave:*Modifcação,saliciladeído,Quitosana*

Highlights

In this work, coordination compounds were obtained and characterized through the reaction of chitosan with salicylaldehyde, with subsequent addition of the metals:Zinc, manganese, and nickel.

Resumo/Abstract

As Bases de Schiff (BS) constituem uma classe de compostos amplamente estudados devido à sua versatilidade nas aplicações, ela é caracterizada pela presença da ligação imina (C=N). Neste trabalho, foram obtidos compostos de coordenação através da formação de uma BS, da reação entre quitosana e salicilaldeído, com posterior adição dos metais: zinco, manganês e níquel. Para a caracterização fez-se uso das técnicas de espectroscopia de UV-VIS, infravermelho, análise termogravimétrica e DRX. Com relação a solubilidade, os compostos foram parcialmente solúveis em solução tampão 5,5 e DMSO. O estudo de espectroscopia na região do UV-Vis realizada em tampão pH 5,5 identificou duas bandas: 255 nm e 325 nm, a primeira relacionada à transição eletrônica $\prod \rightarrow \prod^*$ no anel aromático do aldeído e a segunda a formação da ligação C=N da BS. Não foi possível observar bandas de transição d-d. A espectroscopia na região do infravermelho identificou uma banda característica do estiramento imina (C=N) em aproximadamente 1635 cm^{-1}, confirmando a formação da BS, bem como a presença da banda do anel aromático do aldeído em 1591 cm^{-1}. A comparação entre os espectros da BS e dos complexos metálicos revelou deslocamentos nas bandas características, especialmente na banda de estiramento imina (C=N), cujos valores variaram de acordo com o metal coordenado, sendo o efeito mais pronunciado para o complexo com zinco. Esses deslocamentos fornecem indícios da coordenação metálica, uma vez que a interação do metal com o par de elétrons do nitrogênio da imina altera a densidade eletrônica da ligação C=N, resultando em mudanças nas frequências vibracionais observadas no infravermelho. A análise termogravimétrica indica que os compostos formados com manganês e zinco possuem uma primeira perda de massa superior ao observado para a BS. Segundo o DRX a ordem do índice de cristalinidade (%) observado para as amostras é QP (58,3) > BS (74,3) > Ni-BS (52,4).

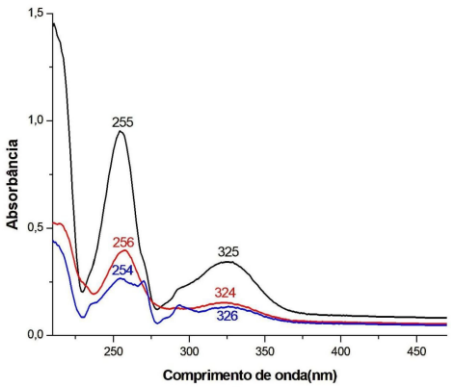


Figura 1-UV-ViS em tampão fosfato pH 5,5 para os metais BS-Zn(Preto), BS-Mn(Vermelho), BS-Ni(Azul).

Agradecimentos/Acknowledgments

A Central Analítica do IQ pelo aporte de equipamentos utilizados nas técnicas de caracterização de UV-Vis e RMN. Ao LABPROBIO, vinculado NUPPRAR/UFRN, pela análise térmica.

Catalytic Activity Studies of the Ce-based MOF and its respective oxide CeO2 (RT) in the Knoevenagel reaction.

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Palavras Chave:*Cerium oxide, Knoevenagel, Green chemistry, Catalyst.,Metal-organic-framework, Cerium oxide, Knoevenagel, Green chemistry, Catalyst*

Highlights

MOF and oxide catalyst based on cesium and succinic acid for Knoevenagel reaction, EtOH:H2O solvent as a green alternative for organic reactions with low reaction times and good yields.

Resumo/Abstract

Metal-organic frameworks, also known as MOFs, are crystalline inorganic solids composed of metal centers interconnected three-dimensionally through coordinated bonds by organic molecules. These materials exhibit high structural tunability and potential application as heterogeneous catalysts. Among C-C bond formation reactions, the Knoevenagel condensation is widely employed in the synthesis of coumarins and related compounds with relevance to cosmetic and pharmaceutical industries [1]. Recent papers have focused on establishing more sustainable catalytic systems for this reaction, emphasizing green solvents and reusable catalysts. This study focused on the catalytic performance of a cerium–succinic acid MOF and its oxide derivative, CeO_2(RT), which were evaluated in the Knoevenagel reaction. The use of cerium oxide was motivated by recent reports on nano-CeO_2 as an efficient catalyst for Knoevenagel. The materials were synthesized at room temperature and its oxide derivative was obtained by calcination at 350°C [2]. The investigated reaction systems were vanillin and malononitrile as substrates and ethanol–water (3:7, v/v) as solvent, following green chemistry principles. Both materials exhibited high catalytic efficiency with 100% conversion under investigated conditions. Significant reductions in reaction time were observed when compared to non-catalyzed systems. Using the oxide catalyst, reaction time was reduced from 4.5 h to only 30 min at room temperature, while the MOF catalyst reduced the reaction time from 75 min to 30 min. Preliminary recyclability studies revealed partial catalyst recovery, with approximately 32% (8 mg from an initial 25 mg) of the initial catalyst mass recovered through a simple filtration system. The catalysts used in this study established a higher efficiency reaction system on Knoevenagel reaction compared to other MOFs previously published.

[1] Tietze, L. F. et al., Comp. Org. Syn., 1991.

[2] Mendes, N. P. A. et al., ACS Omega, 2024.

Agradecimentos/Acknowledgments

We would like to thank the SIAP research group and the Medicinal Organic Synthesis Laboratory of Paraíba (LASOM-PB) for their support, and CAPES, CNPq, FINEP, INCT-CiMol and PROPESQ for their financial support.

Cerium Coordination Polymer with Carboxylate Ligand: Crystal Structure and Electrocatalytic Activity for OER in Neutral Medium

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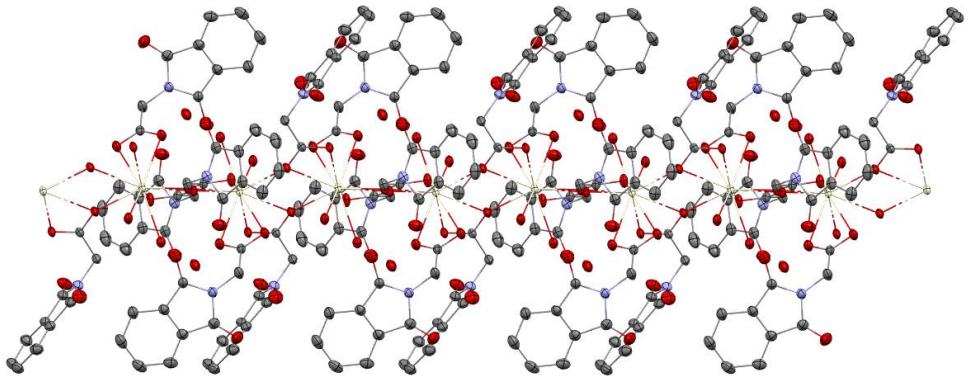
Palavras Chave:*Cerium,Carboxylate ligand,Coordination polymer,OER,Neutral medium*

Highlights

Cerium-carboxylate polymer synthesis and structural elucidation. Investigation of OER activity in neutral medium. Stable and pure crystalline phase as a catalyst platform.

Resumo/Abstract

Hydrogen (H_2) production via water electrolysis is one of the most promising pathways for the energy transition, however, its efficiency is limited by one of the half-reactions involved in the process, the Oxygen Evolution Reaction (OER). Due to this limitation, high-efficiency electrocatalysts are required. In this context, this work reports the synthesis, structural elucidation, and electrocatalytic performance of a new Cerium (Ce^{3+}) coordination polymer based on the carboxylate ligand*N*-phthaloylglycine (phthgly). For the complete characterization of the ligand and the complex, Fourier-transform infrared spectroscopy (FTIR), ^1H and ^{13}C NMR, thermal analysis (TG/DTA), UV-Vis spectroscopy, and X-ray diffraction (XRD), both powder and single-crystal, were employed. FTIR and NMR results denote the successful synthesis of the ligand and its coordination to the metal center. TG/DTA analysis revealed the presence of coordinated and crystallization water molecules in the structure. The crystal structure, resolved by single-crystal XRD, revealed that the compound crystallizes in the triclinic system, space group P-1, organizing as a one-dimensional polymeric chain formed by trinuclear units, presenting the molecular formula $\{[Ce_3(phthgly)_5(H_2O)_2]\cdot H_2O\}_\infty$ (1). The crystalline phase purity shows excellent agreement between the experimental powder diffraction pattern and the simulated pattern from the single-crystal data. OER activity was investigated by electrochemical techniques exclusively in neutral medium (PBS), aiming to address the scarcity of literature data for metal-organic structures under these conditions. In neutral medium, the material exhibited an overpotential of 667 mV (at 10 mA cm^{-2}) and a Tafel slope of 142 mV dec^{-1}. The results indicate that the 1D structure provides a stable platform for catalysis under mild conditions, highlighting the potential of lanthanide polymers as templates for H_2 production in neutral media.



ORTEP of the compound 1 along the a-axis with 30% of probability (all hydrogen atoms omitted)

Agradecimentos/Acknowledgments

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Characterization of the metabolic profile of tumor and non-tumor lung cells exposed to cisplatin by 1H NMR spectroscopy

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Palavras Chave:*cisplatin, NMR metabolomics, HRMAS NMR, MRC-5 cells, A549 cells,cisplatin,NMR metabolomics,HR MAS NMR,MRC-5 cells,A549 cells*

Highlights

^{1}H NMR metabolomics revealed cisplatin-induced metabolic alterations in lung cancer A549 cells, highlighting changes in the histamine, mannose, taurine and threonine metabolites.

Resumo/Abstract

Despite the increasing interest in the development of novel coordination compounds as chemotherapeutics, most of these new complexes are still poorly characterized in mechanistic and metabolic terms, due to their multiple biological targets inside cells, including those in clinical use.[1] In this context, NMR metabolomics represents a powerful tool to characterize the cellular metabolic effects of potential anticancer drugs and to gain a more specific understanding of their mechanism of action. In this work, we investigated the*in vitro*effects cisplatin drug in the metabolism of A549 human lung adenocarcinoma and MRC-5 non-tumoral lung cell lines*in vitro*in response to the cisplatin drug, using High Resolution Magic Angle. ^{1}H NMR metabolomics revealed a higher number of altered metabolites in A549 cells compared to MRC-5 cells.

Specifically, phosphocholine levels were significantly higher in tumor A549 cells, consistent with its role as a tumor biomarker associated with tumor cells transformation and altered membrane metabolism. Further data analysis indicates that a total of 26 metabolites were identified on the A549 cisplatin-treated cells, a total of 8 metabolites were significantly different from the negative control cells (0.5% DMSO). A group of four metabolites was detected in cells exposed to cisplatin, including histamine, mannose, taurine and threonine. These findings suggest dysregulation of amino acid metabolism and carbohydrate metabolism, particularly glycolysis and gluconeogenesis. Alterations in taurine metabolite levels may correlate with the chemosensitizing effects of cisplatin[2]. This work demonstrates that cisplatin treatment has a pronounced effect on the main metabolic pathways in the cancer cell lines. In future studies, ^{1}H NMR metabolomics could be used in investigations to understand the effects of ruthenium complexes on different metabolic pathways.

1. Lamego, I.;*et al.J. Proteome Res.*2014, 13, 12, 6033–6045

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CNPq, CAPES, FAPESP

Circularly Polarized Luminescence of achiral anionic tetrakis lanthanide complexes and chiral cations

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Palavras Chave:*CPL, tetrakis, lanthanides, chirality*

Highlights

Synthesis and characterization of tetrakis complexes of europium(III) with chiral counter-ions; Study of Luminescence and Circularly Polarized Luminescence of these complexes.

Resumo/Abstract

Trivalent lanthanide ion complexes (Ln^{3+}) have been extensively investigated due to their narrow emission bands arising from 4f–4f intraconfigurational transitions, which are largely independent of the coordinated ligands. Chiral lanthanide complexes, particularly Eu(III), enable the detection of circularly polarized luminescence (CPL). CPL corresponds to the spontaneous emission of right- and left-handed circularly polarized light, and the difference between these emission intensities constitutes the CPL spectrum. The practical applicability of such compounds requires simultaneously high $|g_l u_m|$ values (dissymmetry factor) and high emission quantum yields, which remains a central challenge for the development of functional chiral complexes. In pursuit of this goal, this work investigated the luminescence and CPL behavior of achiral anionic Eu(III) tetrakis complexes with high emission quantum yields, in which chirality was induced through cationic protonated chiral amines. The complexes studied were $Na[Eu(tta)_4]$, R/S-MBAH$[Eu(tta)_4]$, and R/S-NEAH$[Eu(tta)_4]$ (tta^- = deprotonated thenoyltrifluoroacetone; R/S-$MBAH^+$ = protonated (R/S)-α-methylbenzylamine; R/S-$NEAH^+$ = protonated (R/S)-1-(1-naphthyl)ethylamine). They were synthesized by coordinated-water replacement of $[Eu(tta)_3(H_2O)_2]$ by tta^-, under microwave conditions and simple stirring, or via cation-exchange reactions using $Na[Eu(tta)_4]$. The chiral complexes were incorporated into poly(ethylene-co-vinyl acetate) (EVA) films. The complexes were characterized by thermogravimetric analysis, mass spectrometry, single-crystal X-ray diffraction, circular dichroism, UV–Vis and FTIR, luminescence, CPL measurements and emission lifetime. The results demonstrated that room-temperature synthesis provides the most efficient route to the chiral amine salt complexes and that no significant interaction occurs between the ligands and chiral cations in solution. EVA films proved to be a promising medium for CPL and CD measurements.

Agradecimentos/Acknowledgments

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Cluster-based redox responsive super-atomic MRI contrast agents

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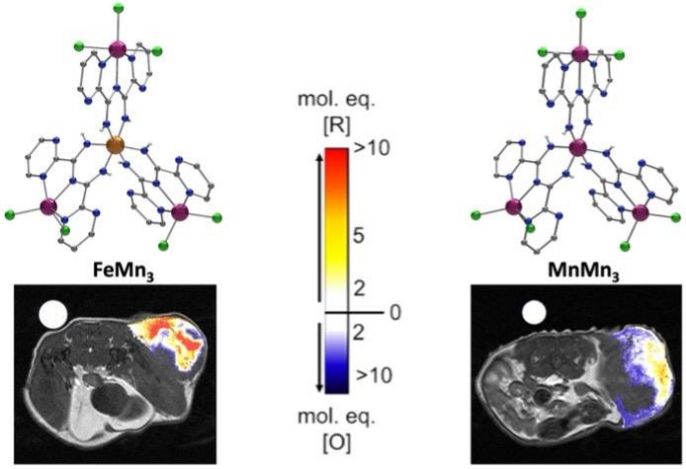
Palavras Chave:*contrast agent design,homo- and heterometallic complexes,magnetic resonance imaging,redox chemistry,contrast agent design,homo- and hetermetallic complexes,molecular imaging,redox chemistry*

Highlights

Polynuclear metal ion complexes with variable oxidation states
Redox-responsive MRI probes
*T*1w/*T*2w ratiometric approach for semi-quantitative*in vivo*MRI of tissue redox status

Resumo/Abstract

Transition metal molecular clusters hold great promise as MRI probes, where careful selection of chemical design elements can afford control over the size, shape and total spin state of the contrast agent molecule. A key characteristic of transition metal molecular clusters that can endow these contrast agents with advanced*in situ*reactivity to biomolecular changes in their environment is that the collection of metal ions within the cluster are linked electronically and can act as a single entity. To date, the potential of transition metal molecular clusters as MRI contrast agents has not been realized due to the problem of cluster dissociation/speciation in biological media. To resolve this challenge, we have employed the*N*-2-pyrimidylimidoyl-2-pyrimidylamidine chelate to selectively bind 3d metal ions to form highly stable mixed metal clusters. This presentation will focus on these biologically stable chelates, in which the microenvironment-responsive chemical activities of our mixed metal clusters enable us to map biochemical redox potentials spanning reducing and oxidizing environments. Via spectroscopic, electrochemical and magnetic analysis along with*in vitro*and*in vivo*studies, the application of iron and manganese homo- and heterometallic triskelion-shaped metal clusters as MRI contrast agents capable of mapping tumor redox status through a simple T_1w/T_2w ratiometric approach will be demonstrated. The contrast agent design strategy presented introduces heteropolynuclear transition metal complexes suitable for semi-quantitative*in vivo*MR imaging of tissue redox status and opens up new avenues for non-invasive characterization of biochemical microenvironments by MRI.



Molecular structures (top) and colour-coded mapping of tumor xenograft redox status (bottom).

Cobalt Coordination Compounds with o-vanillin derived Schiff Base Ligands: Synthesis and Characterization

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Palavras Chave:*Cobalt,Coordination Compounds,Schiff Bases,Vanillin,Biological properties*

Highlights

This work aims to synthesize and characterize*o*-vanillin derived Schiff Base ligands and their cobalt complexes for posterior investigation of their biological properties.

Resumo/Abstract

Thiosemicarbazones (TSCs) are formed by reaction between thiosemicarbazides and aldehydes/ketones, and stand out due to their antifungal, antibacterial, antiviral and antitumoral properties by interacting with RDR enzyme. Vanillin is an aldehyde with antitumoral and antimicrobial activity. Besides, TSCs may be used as ligands in complexes, in which Co stands out as a metal center, showing antitumoral and antibacterial activity. This work aims to synthesize and characterize the o-vanillin derived TSC and its cobalt complex. The TSC-Ph synthesis happened by a reaction between phenylthiosemicarbazide and*o*-vanillin, in acetic acid, 80ºC for 1 hour. Water was added and formed a white precipitate, which was filtered and washed with cold water. The complex synthesis happened by the reaction of the previous ligand with CoCl2.6H2O, in ethanol with 6 HCl drops in reflux for 2 hours. A brown precipitate was obtained and dried in the oven. The NMR ^{1}H showed all signals expected for the TSC: NH (11,78 ppm), OH (9,27 ppm), HC=N (8,52 ppm) and aromatic (6,79 - 7,68 ppm), and MS confirmed it (302,17 g mol^{-1}, positive mode). FTIR allowed placing the main bands for the TSC: 3470 (*ν*OH); 1543 (*ν*C=N) and 831 cm^{-1} (*ν*C=S) and a shift for the complex: 3433 cm^{-1} (*ν*OH); 1575 cm^{-1} (*ν*C=N) and 856 cm^{-1} (*ν*C=S). UV-Vis showed a$\pi^* \leftarrow$ n in 335 nm, as expected for the TSC. Still, the complex spectra showed a CT band in 203 nm with a 255 nm shoulder. CV showed stability of the complex during 20 cycles; a reversible process which suggested a pair Co(II)/Co(III) (0,25 V) and an irreversible process (0,59 V), attributed to TSC. Molar conductivity setted a charge +1 for the complex, suggesting the coordination of Cl$^-$. That way, the analysis confirmed the formation of the TSC-Ph, and suggested the coordination of both TSC and Cl$^-$ in the Co(III) center, being the final complex [Co(TSC-Ph)$_2$Cl$_2$]Cl. More analysis might help elucidate the complex structure, to then have their biological properties evaluated.

Agradecimentos/Acknowledgments

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Complexo binuclear de Cu(II) com ligante aminobis(naftol): implicações estruturais e citotóxicas

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Palavras Chave:*Bioinorgânica,Complexos de cobre,Aminobis(naftol),Superfície de Hirshfeld,Eletroquímica*

Highlights

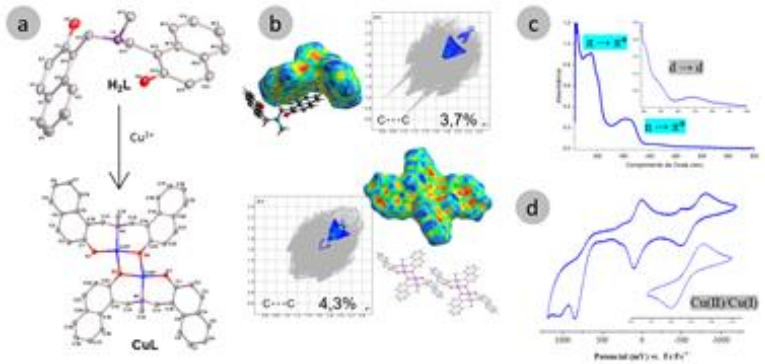
New aminobis(naphthol) ligand with extended π system; Novel binuclear Cu(II) complex exhibiting cytotoxic activity against tumour cells.

Resumo/Abstract

Complexos metálicos binucleares desempenham papéis essenciais em sistemas biológicos, em especial como sítios ativos em metaloenzimas. Na tentativa de mimetizar essas estruturas, novos ligantes multidentados são desenvolvidos1. Neste trabalho é reportada a síntese, caracterização e avaliação da citotóxica de um novo ligante aminobis(naftol), N,N-bis(2-hidroxi-naftilmetil)metilamina (H_2L), bem como de seu complexo de cobre. Resultados de DRX-SC revelam que o ligante coordena-se de forma tridentada $(O,N,O)^{2-}$ ao Cu(II), originando um complexo binuclear quadrado-planar (CuL), com dupla ponte Cu-Oμ-Cu (média 1,9505 Å). Os grupos naftólicos favorecem interações intermoleculares do tipo π···π, importantes no reconhecimento e atividade biológica2, cuja presença é evidenciada nas superfícies de Hirshfeld para o ligante livre (C···C 3,7%) e para o CuL (C···C 4,3%). Diferente de complexos de cobre análogos, o sistema π estendido do CuL influencia no ângulo de torção intermetálico (180o), permitindo a coplanaridade dos átomos de Cu(II). Estudos eletroquímicos evidenciam uma oxidação atribuída ao ligante em potenciais positivos, além do par redox $Cu^{2+}/^{1+}$ ($E_1/_2$ = −987,5 mV, vs Fc0/+, em DMSO) para o complexo CuL. No UV-Vis do CuL (DMSO), transições IL (π→π e n→π*) do H2L aparecem em 288 e 356 nm, respectivamente, além de bandas d-d observadas em 407, 478 e 682 nm. A citotoxicidade avaliada frente às linhagens tumorais humanas HeLa, A549 e MCF-7 através do ensaio de MTT mostram que o ligante e o complexo apresentam efeito citotóxico dependente da concentração, sendo o complexo CuL mais ativo, com valores de IC_{50} entre 28,76 ± 2,01 e 34,68 ± 13,68 μM, enquanto o ligante livre apresentou IC_{50} entre 54,14 ± 0,99 e 63,39 ± 4,32 μM. Os resultados evidenciam o potencial dos complexos com o ligante aminobis(naftol) como uma nova e promissora classe de compostos bioativos.

Matos, C. P. et al. Dalton Trans. 48, 8702–8716 (2019).

Nisbet, M. L. et al. Cryst. Growth Des. 21, 552–562 (2021).



a) Estruturas ORTEP e b) S. Hirshfeld do H2L e CuL, c) UV-Vis e d) Voltamograma cíclico do CuL.

Agradecimentos/Acknowledgments

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Complexos de molibdênio biofílicos multifuncionais com potencial aplicação como estimulantes foliares de fotossíntese

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Palavras Chave:*Química do solo, Complexos de molibdênio, dopamento químico, fotossíntese, nutrição vegetal*

Highlights

O complexo de molibdênio foram sintetizado e caracterizado, e sua estabilidade e efeito como estimulante foliar de fotossíntese foi evidenciado em ensaio em casa de vegetação.

Resumo/Abstract

Devido instabilidades geopolíticas no mundo, é notável a necessidade de novos fertilizantes para promover maior autonomia no agronegócio brasileiro. Por esse motivo, vem se buscando novas alternativas de fertilizantes produzidos em solo nacional. Nesse contexto, compostos de molibdênio, por auxiliarem na fixação de nitrogênio no ar, têm sido aprimorados para reduzir o uso de fertilizantes à base de nitrogênio, que, atualmente, devido à grande população mundial e à necessidade de alimentação, apontam riscos futuros de poluição por nitrogênio. Sendo assim, o objetivo deste trabalho é sintetizar e caracterizar um composto de coordenação com biomoléculas para aplicação foliar e atividade antioxidantes em culturas Pernambucanas. Parâmetros biométricos, análise de nódulos e atividade antioxidantes; avaliação do efeito induzido sobre o processo fotossintéticos, no fortalecimento da parede celular vegetal e nível de nutrição da planta por fixação de nitrogênio. A síntese do composto foi realizada por meio de agitação mecânica por 24h e abrigo de luz. A caracterização do composto foi realizada por meio de espectroscopia de luminescência, de absorção eletrônica e vibracional, e de análise termogravimétrica. A avaliação da atividade antioxidante foi realizada por meio dos testes FRAP, CUPRAC e do nitrato redutase. A formação do composto foi evidenciada pelos sinais característicos das técnicas mencionadas. Os resultados biométricos obtidos com a aplicação do composto indicaram aumento em todos os parâmetros avaliados, e a atividade antioxidante mostrou-se promissora.

Agradecimentos/Acknowledgments

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Comportamento térmico e espectroscópico de nanopartículas de oxalatos de terras raras

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Palavras Chave:*Nanopartículas,Oxidos,Oxalatos,Terras raras*

Highlights

Controlled synthesis of rare-earth oxalate nanoparticles using a slow-release precursor.

Rare-earth oxalates as versatile precursors for morphology-controlled oxides

Resumo/Abstract

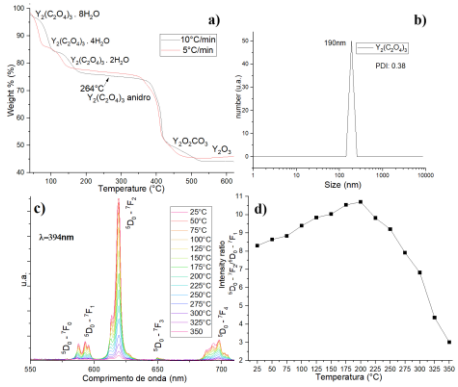
Óxidos de terras raras (TR) são empregados em catálise, iluminação e sensoriamento óptico (Li et al. Discover Appl. Sci, 2025). As rotas de síntese de nanopartículas (NPs) de óxidos requerem decomposição térmica de precursores em temperaturas acima de 500°C ou precipitações em altas pressões ou solventes coordenantes, ambos com controle limitado da morfologia e microestrutura, motivando rotas sintéticas alternativas baseadas em templates ou conversão coloidal. (Rajakumar et al, Appl. Sci., 2021). Este trabalho investiga a síntese de oxalatos (OXs) de TR como NPs coloidalmente estáveis e seu comportamento térmico. Tais partículas são pouco exploradas e podem atuar como precursores para obtenção de óxidos nanoestruturados com preservação da morfologia.

Nesse sentido, NPs de OX de ítrio dopadas com Eu^{3+} foram obtidas por precipitação via hidrólise de oxalato de dietila em solução etanol/etilenoglicol contendo YCl3. As NPs formadas consistem em OXs (Y2(C2O4)3.8H2O) com diâmetro médio de 198±18 nm, mostrando as absorções características de TR2OX3 no infravermelho.

As etapas de decomposição térmica foram investigadas in situ por termogravimetria e por espectroscopia de Eu^{3+}, (25 °C a 350 °C).

O Eu3+ ocupa sítio de baixa simetria (C1) na estrutura monoclínica. As medidas in situ mostram supressão térmica das emissões mesmo com a eliminação das águas de hidratação até ~250°C. Não há alteração significativa no número de componentes das transições 5D0–7FJ, exceto pela diminuição da intensidade da 5D0–7F0, consistente com redução da razão 0-2/0-1, sugerindo aumento da simetria local, menor distorção no sítio metálico ou ocupação de um sítio Ci.

A perda inicial das águas de hidratação não afeta a simetria local do metal, enquanto a saída das águas entre 200 e 300 °C são mais ligadas à esfera de coordenação do Eu3+. Ou seja, 6 águas devem ser estruturais e 2 coordenadas, concordando com os dados de TGA e literatura para Y2(OX)3 bulk (Gribov, et al, Ceramics, 2023).



a)termogravimetria b)DLS das partículas obtidas c)espectros de emissão de Eu3+ e d)razão 7F2/7F1

Agradecimentos/Acknowledgments

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Compostos Nitrosilados de Rutênio com derivados fenantrolínicos

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Palavras Chave:*Nitrosil,Fenantrolina,Rutênio*

Highlights

Synthesis of ruthenium complexes for NO transport. Structural characterization of new nitrosyl species by FTIR, UV-Vis, ^{1}H NMR. Potential application in biological systems.

Resumo/Abstract

O óxido nítrico (NO) é uma molécula diatômica, não carregada e radicalar que é extensamente estudada em decorrência de sua atuação diversa em sistemas biológicos. Participa de processos como vasodilatação (controle da pressão), na coagulação sanguínea (impedindo que as plaquetas se agreguem e impeçam o fluxo sanguíneo), neurotransmissão e no sistema imunológico[1]. O presente trabalho tem como objetivo a síntese, caracterização para posterior aplicação de nitrosil complexos de rutênio (Ru) com derivados fenantrolínicos como potencial transportador de NO. Em um sistema previamente desareado com argônio (Figura 01), obteve-se o óxido nítrico utilizado nas reações através da redução do ácido nítrico diluído pelo cobre metálico, conforme a reação: $8HNO_3(aq) + 3Cu(s) \rightarrow 3Cu(NO_3)_2(aq) + 4H_2O(l) + 2NO(g)$. O NO gerado passa por um sistema de purificação composto por uma solução de KOH concentrada, um frasco contendo sílica e outro contendo cal soldada, com o objetivo de retirar resíduos de vapores de ácido nítrico, umidade proveniente do arrasto de moléculas de água da solução de KOH e possíveis resíduos de NO_2. O NO purificado foi borbulhado em uma solução metanólica de $RuCl_3.3H_2O$ previamente desaerado. Em seguida, à solução resultante de nitrosiltriclororutênio(II), foram adicionados os ligantes 1,10-fenantrolina (phen); 1,10-fenantrolina-5,6-diona (phen_diona) e 5,6-epóxi-5,6-dihidro-1,10-fenantrolina (phen_epoxi). As caracterizações dos complexos formados foram realizadas utilizando RMN de ^{1}H, UV-Vis e FTIR. Os espectros de FTIR apresentaram bandas intensas de ν(NO) em 1878, 1890 e 1901 cm^{-1} e ν(C=N) na faixa de 1440 - 1429 cm^{-1}, enquanto o UV-Vis revelou transições entre 354 e 493 nm. Os deslocamentos químicos de RMN ^{1}H estão de acordo com o esperado e calculado e com as seguintes propostas estruturais $Ru(phen)(Cl)_3(NO)$; $Ru(1,10\text{-}phen_diona)_2(Cl)(NO)$ e $Ru(phen_epóxi)(Cl)_3(NO)$.

1 - TOLEDO, J.C.; AUGUSTO, O. Chem. Res. Toxicol., v. 25, p. 975, 2012.

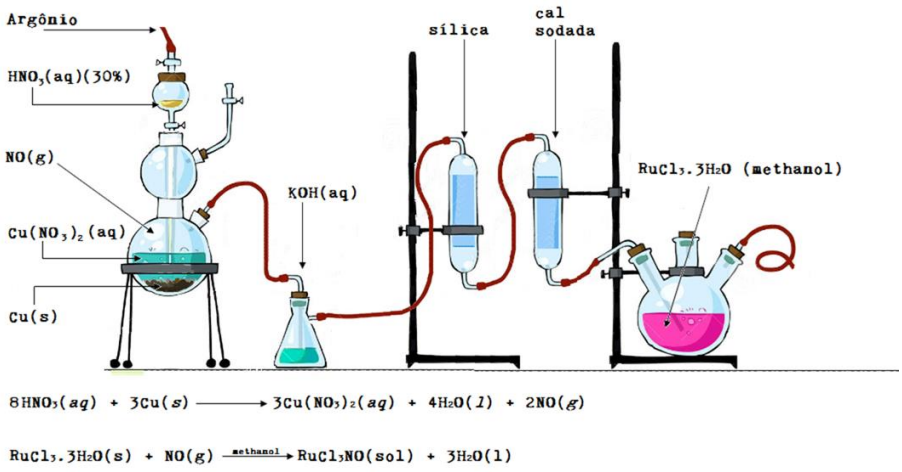


Figura 1. Sistema de geração e purificação de NO.

Agradecimentos/Acknowledgments

Petrobras-CENPES; IMQ-UFRJ

Computational Insights in Merocyanine-Based Lanthanide Complexes

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Palavras Chave:*Lanthanides,Merocyanine,NIR emission,Computational Chemistry,Antenna effect*

Highlights

Ln–O distances indicate coordination asymmetry in LnMC complexes. Merocyanine ligands act as antennas, and NIR emission depends on ligand–metal spectral separation.

Resumo/Abstract

Lanthanide complexes emitting in the near-infrared (NIR) are of interest for photonic and sensing applications, but their weak direct absorption requires efficient antenna ligands [1]. In this work, a series of lanthanide complexes composed of a central Ln^{3+} ion coordinated by two merocyanine (MC) ligands and nitrate groups (LnMC; Ln = Nd, Eu, Tb, Tm, Yb) was investigated.

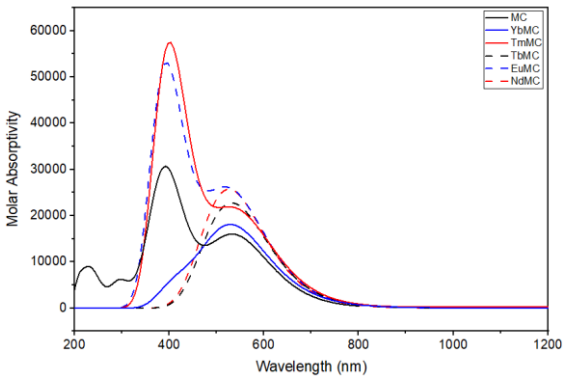
Geometry optimizations and frequency calculations were performed at the UB3LYP/cc-pVDZ level with SDD relativistic effective core potentials for the lanthanides. The optimized structures reveal asymmetric coordination, with dominant metal–ligand interactions involving phenolate oxygen atoms of the MC units. Time-Dependent Density Functional Theory (TD-DFT) excited states were computed at the B3LYP level using the same basis set scheme. The most intense transitions are concentrated in the UV–Vis region and are predominantly π–π* in character, localized on the MC ligands [2]. In contrast, lanthanide-centered excited states associated with NIR emission display very low oscillator strengths, consistent with the forbidden nature of 4f–4f transitions [1].

Low-energy NIR states are predicted for all complexes; however, observable NIR emission is expected only for NdMC, TmMC, and YbMC, whose characteristic emitting levels fall in the NIR range, where the MC ligands do not absorb significantly. For EuMC and TbMC, metal-centered emission occurs in the visible region, overlapping with strong merocyanine absorption and favoring competitive deactivation pathways.

These results suggest that the mere presence of NIR electronic states is not sufficient to ensure lanthanide luminescence, efficient emission depends on spectral separation between ligand absorption and metal emission, as well as on structural factors that modulate energy transfer and non-radiative decay pathways.

[1] Li, J. et al., Discover Applied Sciences, 2025.

[2] Pugachev, A. D. et al., Spectrochimica Acta Part A, 2020.



TDDFT-calculated UV–Vis absorption spectra of the free merocyanine (MC) and the LnMC complexes

Agradecimentos/Acknowledgments

The authors acknowledge the financial support from CNPq and FAPEMIG, and thank UNIFEI and IFQ for institutional support.

Computational Insights of Pt(IV) Complexes Reduction

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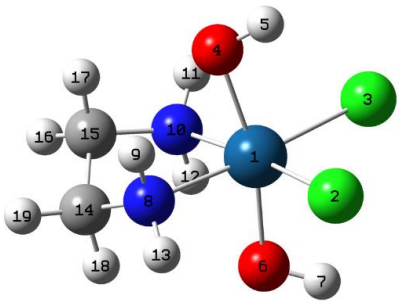
Palavras Chave:*Platinum (IV) Complexes,Implicit Solvation,Thermodynamic Data*

Highlights

The ΔG_r for reduction of c,t-[Pt(en)Cl_2($OH)_2$] are more negative for the equatorial ligand dissociation. Implicit solvation in water favors axial ligand dissociation to a greater extent.

Resumo/Abstract

Reduction of Pt(IV) complexes involves the uptake of two electrons within release of two ligands[1]. This process is irreversible, and consistently related to the axial ligands exit, however, there is evidence indicating the release of equatorial ligands also[1]. In this work, computational calculations were carried out at the MP2 and DFT/M06-2X for the complex c,t-[Pt(en)Cl_2($OH)_2$] and its possible reduction products, considering either the loss of equatorial chlorides or axial hydroxides, in the gas phase (GP), IEFPCM-UFF, and SMD. As shown in the Figure, that include thermodynamic data in the GP only the loss of chlorides has ΔG_r<0 at both levels of theory. Under implicit solvation, all reactions are favored toward the products with maximum differences of 214.47 and 148.17 kcal·mol^{-1} for hydroxide and chloride release in GP, respectively. Thereby, interaction with the dielectric medium favors axial ligand exit to a greater extent, although the ΔG_r remains higher. From the data, it can also be observed that calculations using the SMD model yield a lower free energy for hydroxide release upon reduction, whereas IEFPCM predicts the lowest free energy for chloride release. This probably is related to the larger contribution of hydrogen-bonding in the exit of axial ligands. In addition, differences of 37 to 41 kcal·mol^{-1} were observed between the ΔG_r values calculated at the employed levels of theory, with more negative energies obtained with DFT, possibly due to charge imbalance between products and reactants. In view of this, to reduce the effects of charge and to better understand the structural relationships between solute and solvent, calculations in water with explicit solvation via Monte Carlo simulations will be performed. In addition, reduction potentials will be calculated using the Nernst equation. The same set of calculations will also be carried out for the complex c,t-[Pt(en)Cl_2($OCOCH_3)_2$]. [1] Gibson, D. Dalton Transactions, 2009(48): p. 10681-10689.



	Loss of chlorides			Loss of Hidroxydes		
Solvation	ΔH_r (kcal.mol^{-1})	$T\Delta S_r$ (kcal.mol^{-1})	ΔG_r (kcal.mol^{-1})	ΔH_r (kcal.mol^{-1})	$T\Delta S_r$ (kcal.mol^{-1})	ΔG_r (kcal.mol^{-1})
MP2 – Gas Phase	-11.87	17.94	-29.81	116.97	20.58	96.39
MP2 – SMD	-151.82	17.14	-168.96	-97.82	20.26	-118.08
MP2 – IEFPCM	-161.10	16.88	-177.98	-64.29	20.28	-84.57
M06-2x – Gas Phase	-52.28	18.00	-70.29	77.49	21.11	56.38
M06-2x – SMD	-192.00	17.38	-209.38	-135.15	20.72	-155.86
M06-2x – IEFPCM	-201.16	17.00	-218.17	-102.61	20.80	-123.42

Optmized structure and thermodynamic data (298.15K and 1atm) of c,t-[Pt(en)Cl_2($OH)_2$].

Agradecimentos/Acknowledgments

We want to express our sincere gratitude to CAPES, FAPEMIG, CNPQ, UNIFEI, and IFQ.

Coordination of cobalt (II) with 2-aminophenol via a mechanochemical and solvent-free method

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Palavras Chave:*Co(II) complexes Spectroscopy, Green Chemistry, Mechanochemistry.,Co(II) complexes, Spectroscopy, Green Chemistry, Mechanochemistry.*

Highlights

This abstract describes a mechanochemical synthesis of a the Co(II) complex using 2-aminophenol as a ligand. The spectroscopic data suggests coordination of the ligand with the metal center.

Resumo/Abstract

The concern with sustainable synthetic methods is one of the greatest contemporary concerns, leading to the adoption of methodologies that aim to minimize environmental impacts. In chemistry, green chemistry stands out, seeking to reduce or eliminate waste generation, with mechanochemistry being a methodology aligned with these principles by employing mechanical energy to promote chemical reactions. In this context, this study aimed to synthesize the $[Co(L_1)_2Cl_2].2H_2O$ complex from the 2-aminophenol (L_1) ligand and $CoCl_2.6H_2O$ using the mechanochemical method. The synthesis was performed in a mortar and pestle for 30 minutes, followed by extraction with water, drying, and recrystallization in water/ethanol. The formation of the complex was confirmed by infrared spectroscopy, based on the shift of characteristic bands of the ligand after coordination with the ion. A broad band was observed between 3350–3100 cm^{-1}, attributed to hydration water, as well as bands associated with angular deformations of the metal-oxygen (Co-O) bond between 574-609 cm^{-1} and metal-nitrogen (Co-N) between 588-590 cm^{-1}. The deformations indicate the complexation of the metal to the ligand. The UV-Vis spectrum of the $[Co(L_1)_2Cl_2].2H_2O$ complex showed absorptions at 250 nm ($^2Eg \rightarrow {}^2A_2g$), 340 nm ($^2Eg \rightarrow {}^2A_1g$ (G)), 640 nm ($^2Eg \rightarrow {}^2T_2g$ (G)), and 820 nm ($^2Eg \rightarrow {}^2T_1g$ (G)). The Racah B and C values were 714 cm^{-1} and 2857 cm^{-1}, respectively, with $\Delta o = 16145\ cm^{-1}$ and $\beta = 0.70$, indicating that the L_1 ligand (2-aminophenol) favors a possible strong field with a low spin configuration. Density Functional Theory (DFT) conformational analyses of the complex are underway to elucidate the nature of the observed electronic transitions and to identify any possible charge transfer mechanism. Thus, the results demonstrate that the mechanochemical method is an efficient and environmentally friendly alternative for the synthesis of Co(II) complexes, in accordance with the principles of green chemistry.

Agradecimentos/Acknowledgments

Universidade Federal Rural de Pernambuco (UFRPE), Universidade Federal de Pernambuco (UFPE), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Fundação de Amparo à Ciência e Tecnologia de Pernambuco (FACEPE) e University of Leeds.

Cytotoxic activity and theoretical–experimental study of the interaction of Ru(II) organometallic complexes with biomolecules.

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Palavras Chave:*ruthenium(II),leukemia,DNA,BSA,fluorescence.*

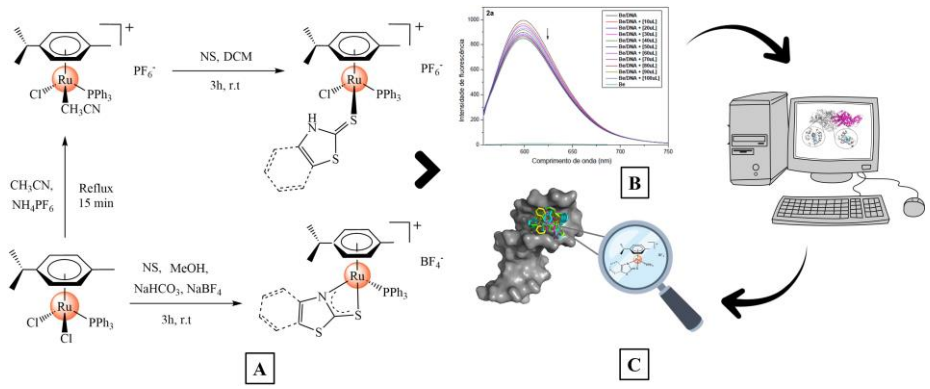
Highlights

Four complexes $[Ru(p\text{-cymene})(PPh_3)(N–S)]^+$ were synthesized and had their structures solved by XRD. The complexes showed affinity for BSA and DNA, as well as cytotoxic activity against K562 cells.

Resumo/Abstract

In this work, four arene ruthenium complexes containing triphenylphosphine and N,S-donor ligands: 2-mercaptothiazoline (HLa) and 2-mercaptobenzothiazoline (HLb) were synthesized. The compounds were characterized by ^1H and $^{31}P\{^1H\}$ NMR spectroscopy, vibrational and electronic spectroscopy (IR and UV-vis), mass spectrometry, and molar conductivity measurements. For the complexes $[Ru(\eta^6\text{-p-cymene})(L\text{-}\kappa^2N,S)PPh_3]BF_4$, single crystals suitable for X-ray diffraction were obtained. $^{31}P\{^1H\}$ NMR studies in different solvents confirmed the instability of the series 1 complexes ($[Ru(\eta^6\text{-p-cymene})(HL\text{-}\kappa S)PPh_3]BF_4$), except in dichloromethane and chloroform. For the series 2 complexes ($[Ru(\eta^6\text{-p-cymene})(L\text{-}\kappa^2N,S)PPh_3]BF_4$), interactions with DNA and BSA were investigated by fluorescence spectroscopy. Competition assays with ethidium bromide indicated the absence of DNA intercalation, with low binding constants ($K_b \approx 10^2$) and Stern–Volmer constants ($K_{SV} \approx 10^3$). Molecular docking simulations corroborated these findings, indicating preferential interaction within the minor groove, with binding energies ranging from −6.30 to −7.23 kcal mol^{-1}. Regarding BSA, titration assays demonstrated strong affinity, with association constants (K_a) on the order of 10^5 to 10^6 and K_{SV} values of 10^5, suggesting a dynamic interaction mechanism. Thermodynamic calculations revealed that van der Waals forces and hydrogen bonding dominate for complex**2a**, whereas hydrophobic interactions prevail for**2b**, with interaction energies between −6.56 and −8.49 kcal mol^{-1}. The analyses indicate that the complexes interact with DNA and BSA at a single active site.

Preliminary cytotoxic activity data against chronic myeloid leukemia cells (K562) showed promising results, with IC_{50} values ranging from 6.11 to 7.01 µM. These findings highlight the potential of the synthesized complexes as pharmacological candidates, emphasizing their ability to interact with biomolecules and their antitumor activity.



A: Synthetic route of the "Ru–arene" complexes; B: "Ru–DNA" interaction; and C: Molecular docking.

Agradecimentos/Acknowledgments

I acknowledge the Federal University of Santa Catarina (UFSC), the Graduate Program in Chemistry (PPGQ), and the funding agencies for the institutional and financial support that enabled the development and execution of this research work.

Desenvolvimento de novos complexos de cobre(II) e cobalto(II) com ligante vaniloide

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Palavras Chave:*Cobre(II),Cobalto(II),Apocinina,Antitumoral*

Highlights

New copper(II) and cobalt(II) complexes with apocynin ligand. Characterization by SC-XRD, IR, UV-Vis and cyclic voltammetry.
Search for new coordination compounds with antitumor activity.

Resumo/Abstract

Compostos de coordenação são utilizados como metalofármacos no tratamento de diferentes enfermidades, incluindo o câncer. Cobre e cobalto são metais essenciais para o organismo humano, onde o cobre atua como centro redox em diferentes metaloenzimas enquanto o cobalto encontra sua atividade relaciona principalmente à composição da vitamina B12. Estes metais têm sido utilizados no desenvolvimento de novos complexos com atividade biológica[1]. A apocinina (Hapo) apresenta um grupo vanilóide e que possui atividade de inibição da enzima NADPH-oxidase. Este trabalho aborda a síntese e caracterização de novos complexos *trans*-$[M(H_2O)_2(apo)_2]$, onde M representa os íons Cu(II) (1) e Co(II) (2) tendo o íon apocinina (apo) como ligante. A difração de raio-X do complexo de 1 (Fig. 1) revelou uma geometria octaédrica com dois íons apo coordenados ao metal e posicionados em trans, com comprimentos de ligação 1,931 Å (Cu-$O_{(fenóico)}$) e 2,310 Å (Cu-$O_{(metóxido)}$). Nos espectros de infravermelho a banda de vC=O encontrada no Hapo em 1657 cm^{-1} foi deslocada para 1629 cm^{-1}(1) e 1631cm^{-1}(2), evidenciando a coordenação. A ausência da banda vO-H fenólico, confirma a deprotonação do íon apo nos complexos. Os espectros Uv-Vis dos complexos apresentam bandas π-π* do íon apo em 276 e 303 nm. O complexo de Cu^{2+} apresenta ainda três transições d-d em 464, 784, 911 nm, decorrentes da distorção tetragonal. Já para o composto de Co^{2+}, observou-se duas bandas d-d de maior intensidade em 496 e 628 nm e quatro outras bandas com menor intensidade, provavelmente duplamente proibidas. A voltametria do complexo 1 revelou um potencial de meia onda ($E_1/_2$) de 173 mV, referente ao para redox $Cu^{2+}/^{1+}$ e um processo irreversível da redução $Cu^{1+}/^{0}$ em -463 mV. Já o complexo 2 possui um processo irreversível em 122 mV ($Co^{2+}/^{1+}$), e processo de oxidação do ligante apo. Assim, os resultados confirmam a obtenção dos compostos de interesse.

[1]Adhikari, S.,et al., Biomedicine and Pharmacotherapy, 171, 2024, 116211.

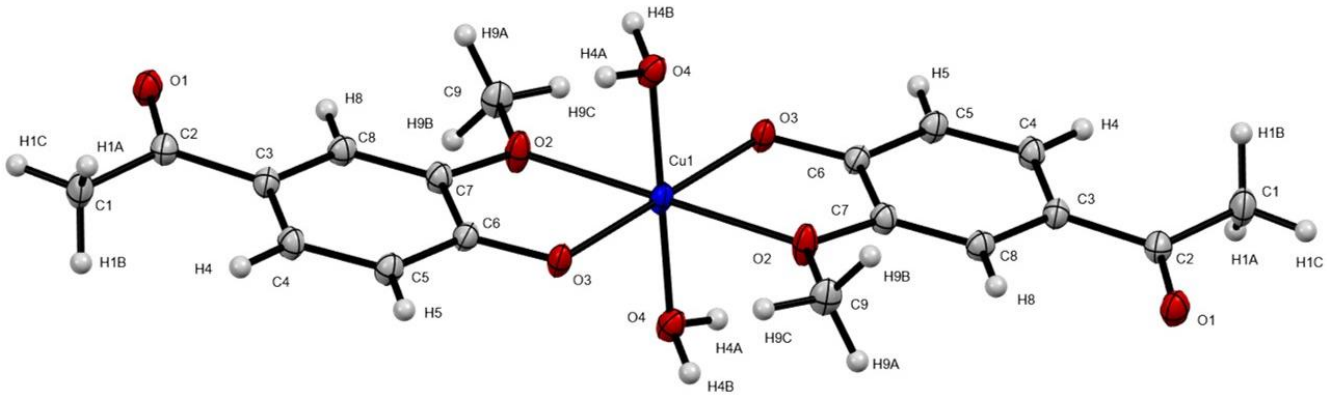


Figura 1. Estrutura ORTEP do composto 1.

Agradecimentos/Acknowledgments

UFRN, LQCPol.

Desenvolvimento de um novo complexo de cobalto(III) com ácido kójico

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Palavras Chave:*Compostos de coordenação,Cobalto,ácido kójico.*

Highlights

A novel cobalt(III) coordination compound combining the properties of 1,10-phenanthroline and kojic acid ligands;

Search for new coordination compounds with antitumor activity.

Resumo/Abstract

Compostos de coordenação de cobalto(III) tem despertado interesse quanto a sua potencial atividade antitumoral. Em particular, complexos contendo ligantes auxiliares planares, tal como 1,10-fenantrolina (phen), que podem favorecer a intercalação com o DNA.[1] O ácido kójico (Hka) é produzido por espécies de fungos a partir de processos fermentativos, sendo utilizado no tratamento de melasmas, atuando como inibidor da tirosinase. Adicionalmente, apresenta também propriedades antimicrobianas e antifúngicas.[2] Este trabalho tem como objetivo a síntese e caracterização dos complexos $[Co(phen)_2(Cl)_2]Cl$ e $[Co(phen)_2(ka)](PF_6)_2$, identificados como CoPCl e CoPK, onde ka corresponde ao íon kójico. A estrutura de raio X do complexo CoPK (Fig. 1) revelou comprimentos de ligações médios Co-N e Co-O iguais a 1,945 e 1,900 Å, respectivamente, e ângulo de ligação axial N-Co-N de 177,3°, evidenciando um ambiente de coordenação octaédrica N_4O_2. Os espectros de IV do CoPK exibiu modos vibracionais vC=C em 1584 cm^{-1} e 1520 cm^{-1}, vC=$N_{(phen)}$ em 1461 cm^{-1} e 1431 cm^{-1}e a banda vC=Oem 1546 cm^{-1}, referentes ao íon kójico, confirmando sua presença na esfera de coordenação. Os espectros de Uv-Vis apresentaram bandas d-d para o complexo CoPCl em 534 e 612 nm. Já para CoPK, estas transições observadas em 471 e 572 nm. A variação observada para CoPK evidencia a alteração de energia dos orbitais envolvidos nas transições devido a coordenação do íon kójico. Os valores de $E_1/_2$ para o processo redox $Co^{3+}/^{2+}$ para os compostos CoPCl e CoPK foram encontrados em 128 e 135 mV respectivamente, a variação para maiores valores dos potenciais de meia onda mostra que houve a mudança na densidade eletrônica do metal o tornando mais deficiente eletronicamente. Assim, os resultados confirmam a obtenção dos compostos de interesse.

[1]WANG, Xiang Li et al. Journal of Inorganic Biochemistry, 98, 6, 2004. [2]BRTKO, Julius. Archiv der Pharmazie, Weinheim, 355, 10, 2022.

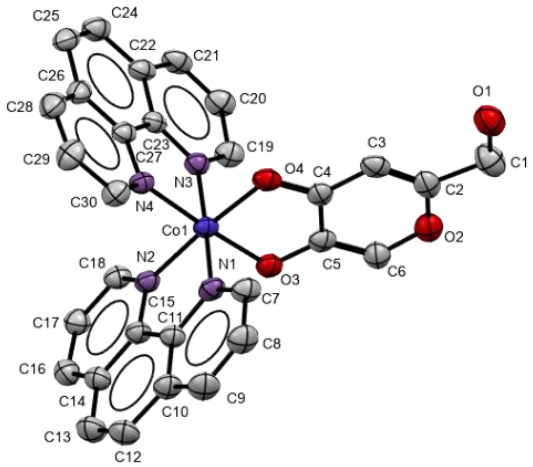


Figura 1. Estrutura cristalográfica do complexo CoPK

Agradecimentos/Acknowledgments

UFRN, LQCPol, LaMuCrEs - IFSC/USP

Development of a low-cost magnetic susceptibility measurement instrument using 3D printed parts

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Palavras Chave:*Magnetic susceptibility,instrumentation,3D printed Instruments,open source,coordination compounds*

Highlights

A low-cost, open-source magnetic susceptibility device was made for under R$ 150. Used to qualitatively demonstrate magnetic susceptibility of different paramagnetic coordination made at UFRJ course

Resumo/Abstract

Magnetic susceptibility, a material's intrinsic response to an applied magnetic field, is conventionally measured with high precision using magnetometers like the SQUID (Superconducting Quantum Interference Device). However, the prohibitive cost of such equipment often limits its availability. A more budget-friendly approach is the Gouy-Evans balance method, which measures the change in a sample's weight when subjected to an inhomogeneous magnetic field using an analytical balance. Despite its versatility across fields like geology, medicine, and chemistry, commercial Gouy-Evans balances still cost around $650 USD, hindering acquisition for universities in the Global South. To address this accessibility issue, this project developed a low-cost, open-source magnetic susceptibility device. The design incorporates an ESP32 microcontroller for programming and 3D-printed mechanical structures, employing Halbach arrays to enhance measurement sensitivity. The developed device records sample mass variations of few milligrams when subjected to a magnetic field. To maximize this response, the system was optimized by adjusting magnet dimensions, inter-magnet spacing, and the height of the sample into the magnetic field. This setting resulted in the equation: y (mass reading) = 55,4 * e^(-0,297 * x {magnetic field intensity}) with an R2 of 0.978 when varying the magnetic field applied in the sample, thus confirming the exponential relation expected. This device proved being capable to qualitatively demonstrates the magnetic susceptibility of ferroamagnetic, paramagnetic and diamagnetic substances by measuring triplicates of metallic cobalt powder, Mohr's salt and [Fe(bipy3)]2+, respectively during the Experimental Inorganic Chemistry II course at UFRJ.



First prototype made using two parallel permanent magnets and a 0.01 g commercial balance.

Agradecimentos/Acknowledgments

FAPERJ, Studio 42 Tech and UFRJ

DEVELOPMENT OF NEW BINUCLEAR PLATINUM(II) COMPLEXES: SYNTHESIS, CHARACTERIZATION, AND CYTOTOXICITY.

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Palavras Chave:*Cancer, nDNA interaction, platinum, chemotherapy.*

Highlights

A novel dinuclear Pt(II) complex was synthesized and characterized. It showed over 90% cytotoxicity in lung, leukemia and colon cancer cells. Strong DNA binding and low toxicity (DL_{50} 300 mg kg^{-1}).

Resumo/Abstract

The clinical use of platinum(II)-based drugs is limited by multidrug resistance (MDR), which consists of an adaptive process that allows tumor cells to survive different therapeutic regimens. As a result, new chemical approaches are required[1]. In this context, fourth-generation multinuclear platinum(II) systems have been investigated for exploiting alternative modes of interaction with nDNA, resulting in greater antitumor activity and lower toxicity[2]. This work describes the synthesis and characterization of the binuclear complex [Pt(Cl)(en-κ²N)μ-(4,4′-dipy-κ²N)PtCl(en-κ²N)]Cl_2, in which 4,4′-bipyridine acts as a bridging ligand between two Pt(II) metal centers, and 1,2-diaminoethane acts as a terminal ligand. The structure was confirmed by infrared, UV–Vis, and RMN (^{1}H, ^{13}C, and ^{195}Pt) spectroscopy, as well as high-resolution mass spectrometry. Cytotoxic activity was evaluated in vitro by the MTT method against the human tumor cell lines NCI-H292, HEp-2, HL-60, and HT-29. The binuclear complex exhibited high antitumor activity, with cell inhibition percentages above 90%, standing out against lung carcinoma and leukemia models. Thermal denaturation studies of nDNA indicated an increase in melting temperature, suggesting the formation of stable interstrand cross-links capable of hindering biochemical repair and favoring the induction of apoptosis[3]. Acute in vivo toxicity revealed an LD_{50} of 300 mg kg^{-1}, classifying the complex in OECD Category 3, a value higher than that observed for cisplatin, which is classified in Category 1. In addition, hematological parameters remained within reference values, indicating good systemic tolerance. These results demonstrate that the binuclear complex exhibits high potential as a fourth-generation antitumor agent, combining high cytotoxic efficacy with an improved safety profile.

Agradecimentos/Acknowledgments

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Development of Starch-Based Biofilms and Cerrado Resins for PPE: A Preliminary Spectroscopic Study CONVERTIK×

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Palavras Chave:*FTIR, Cassava Starch, Lobeira, Cerrado Resins, Technical Biofilms.*

Highlights

FTIR spectroscopic analyses. The starch has a high amylose content, which allows for future applications of Solanum lycocarpum. Strategy for water-insoluble elastomeric EPI using native resins.

Resumo/Abstract

This work investigates the synthesis of polymeric biofilms with elastomeric properties, using cassava starch as a high-amylose precursor in a proof-of-concept for the future use of lobeira starch (Solanum lycocarpum). The central focus is the development of materials for environmental applications and Personal Protective Equipment (PPE), integrating native vegetable resins from the Cerrado biome to provide water insolubility. FTIR (Fourier-Transform Infrared) characterization was crucial to validate the matrix integrity. The spectra revealed intense bands in the**3300-3500 cm^{-1}**region, indicating hydroxyl group (-OH) stretching and the formation of hydrogen bond networks between the starch and the plasticizer. Peaks at approximately**1015-1080 cm^{-1}**(C-O-C and C-O-H stretching) confirm the reorganization of amylose chains after gelatinization, which is essential for film stability. Spectroscopic analysis suggests that the matrix possesses active sites for the incorporation of hydrophobic resins, justifying the observed reduction in water solubility and the potential for elastomeric behavior. This preliminary study validates the casting technique and molecular analysis, establishing the foundation for replacement with lobeira starch, which, due to its superior polymeric density, will enhance the robustness required for sustainable technical materials.

CONVERTIK×

Agradecimentos/Acknowledgments

Agradecimentos/Acknowledgments: To the Federal University of Catalão (UFCAT) for laboratory support and the use of infrared analytical tools, which were fundamental for the chemical characterization of this biopolymer.

CONVERTIK×

Effect of manganese substitution on the structural properties and electrocatalytic behavior of MOF-derived LaFeO3 perovskites: preliminary analysis

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Palavras Chave:*Clear energy,Hydrogen,Perovskites,Manganese,Electrocatalysis*

Highlights

$LaBO_3$ Perovskites with partial substitution of B-site cations have promising results as electrocatalysts. What effects does the manganese substitution have on $LaFeO_3$'s electrocatalytic behavior?

Resumo/Abstract

The impacts of the climate change led to the seek for alternative energy sources, and, among them hydrogen gas (H_2) stands out. This gas can be obtained via water electrolysis. However, the anodic reaction named Oxygen Evolution Reaction (OER) demands electrocatalysts due to the high energy and slow kinetics, being the main bottleneck in the process. For example, Kalubarme*et al.*reported a $LaBO_3$ perovskite, with partial substitution of the B site by transition metals, that showed promising overpotential [1]. Thus, in this work it is investigate how the distortion of the local symmetry of the $LaFeO_3$ (LFO) crystal lattice, induced by the incorporation of manganese ions (Mn^{2+}), can influence the electrocatalytic performance. The oxides were obtained in two steps: preparation of MIL-100 Metal-Organic Framework (MOF) gels containing 10% and 30% (Mn w/w), followed by thermal conversion at 700 °C for 3 hours. Three samples were synthesized: LFO, LFO/Mn10% (Mn10), and LFO/Mn30% (Mn30), and characterized by X-ray diffraction (XRD) and infrared spectroscopy (FTIR). OER electrocatalytic performance was investigated using linear sweeping voltammetry (LSV) and cyclic voltammetry (CV). The diffractograms confirmed the formation of perovskites with a predominantly orthorhombic structure, corroborated by Rietveld refinement in the GSAS-II software. The peak shifts observed in vibrational spectra indicated the insertion of manganese ions into the LFO crystal lattice. LSV showed overpotentials of 379 mV and 367 mV, and Tafel slopes of 75 $mV \cdot dec^{-1}$ and 78.6 $mV \cdot dec^{-1}$ for Mn10 and Mn30, respectively. CV was used to determine differential capacitances (CDL) of Mn10 and Mn30, which are 2.98 $mF \cdot cm^{-2}$ and 2.986 $mF \cdot cm^{-2}$. These results indicate that the compounds were successful obtained and both Mn10 and Mn30 have promising potential for application as electrocatalysts for OER.
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Agradecimentos/Acknowledgments

The authors would like to thank to CAPES, CNPq, CETENE and FACEPE.

Effects of Electrochemically Generated Cyanide Vacancies in Prussian Blue Electrocatalysts on the Water Oxidation Efficiency in Mild Conditions.

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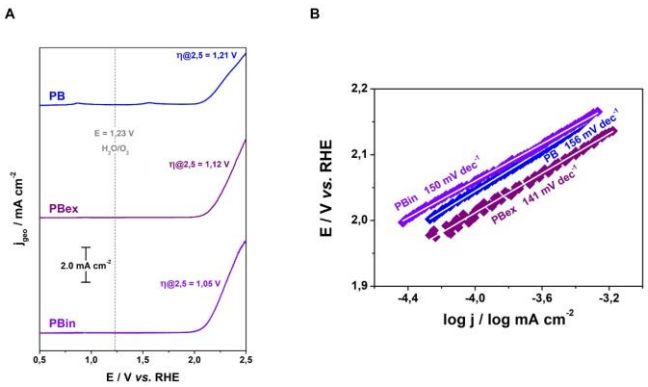
Palavras Chave:*Electrochemical,water oxidation,oxygen evolution reaction,Prussian blue,cyanide vacancies.*

Highlights

Prussian blue analogues were prepared along with CN vacancy. These were produced via in and ex situ electrochemical routes, resulting in better electrochemical parameters for OER under mild conditions.

Resumo/Abstract

Currently, about 95% of the H_2 produced worldwide is derived from coal and natural gas, which are finite resources, and involves a process that releases a large amount of CO_2 into the atmosphere. Only about 5% of H2 production can be considered “green”. Green H_2 produced via water splitting is a promising candidate in this transition. However, the efficiency of this process is limited by the oxygen evolution reaction (OER), where the development of a robust high-performance anode catalysts remains a critical challenge. The OER is a complex reaction involving a transfer of 4 protons and 4 electrons. In this work, we focus on investigating the effects of electrochemically generated cyanide (CN) vacancies in Prussian Blue (PB) electrocatalysts for OER under mild conditions. The materials were electrochemically synthesized on fluorine-doped tin oxide (FTO) substrates. A strong deep blue color was observed over the substrate, indicating successful synthesis of PB. CN vacancies were electrochemically produced during PB preparation (in situ approach – PBin) and as a post treatment procedure (ex situ approach – PBex). Raman spectroscopy revealed typical cyanide bonds-related vibrational modes. Scanning electron microscopy of PB confirmed the presence of cubic particles, while the CN vacancy-containing samples showed particles with poorly defined morphologies. Electrocatalysis tests in 0.1 M KNO^3 solution showed that the overpotentials to achieve 2.5 mA cm^{-2} current density for OER were 1.21, 1.12, and 1.05 V for PB, PBex, and PBin, with corresponding Tafel slopes of 156, 141, and 150 mV dec^{-1}, respectively. These analyses indicate that the two materials with induced CN vacancies exhibited better electrocatalytic activity compared to the traditional PB, and, although both in situ and ex situ samples presented close overpotential values for OER, the PBex has shown a faster and favorable kinetic pathway.



(A) Linear sweep voltammetry of the materials in 0.1 M KNO3 solution and (B) respective Tafel Slopes

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Electronic and structural properties of Ru II complexes with NS ligands and p-substituted triarylphosphines

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Palavras Chave:*ruthenium(II),triarylphosphine,mercaptobenzothiazoline,NS ligand*

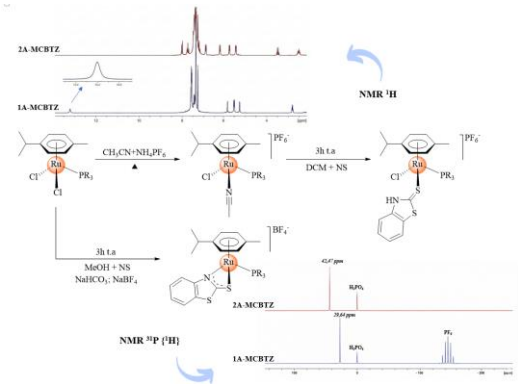
Highlights

Eight complexes were isolated with variations in phosphines and NS ligand coordination mode.

^{31}P NMR indicates higher electron density in monodentate phosphorus complexes than in bidentate ones.

Resumo/Abstract

This study investigated how the coordination mode of the NS Ligand mercaptobenzothiazoline (MCBTZ) influences the electronic properties and reactivity of ruthenium(II) complexes with p-substituted triarylphosphines. A total of eight complexes were isolated in a mono- or bidentate fashion for the NS ligand, leading to two series of complexes with the general formulas [Ru(η⁶-p-cymene)(κS-MCBTZ)(P{Ph-R}$_3$)Cl]PF_6 and [Ru(η⁶-p- cymene)(κ²N,S-MCBTZ)(P{Ph-R}$_3$)]BF_4 (R = OMe, Me, H, and F). Spectroscopic characterization by FTIR and NMR (^{1}H and ^{31}P{^{1}H}) confirmed the structures of these complexes and distinguished their coordination modes, with the presence or absence of the NH signal of the MCBTZ ligand in the ^{1}H NMR spectra serving as a diagnostic indicator of whether the NS ligand was bound in mono- or bidentate fashion, and FTIR bands supporting these assignments. Furthermore, ^{31}P{^{1}H} NMR data revealed systematic variations in the phosphorus chemical shifts as a function of the para substituent on the triarylphosphine, with shifts increasing in the order OMe < Me < H < F, indicating measurable differences in electronic density at the metal center associated with phosphine substitution. Reactivity studies in coordinating solvents showed that complexes with bidentate NS ligands undergo distinct substitution behavior compared to their monodentate analogues, consistent with stronger metal– ligand interactions in the bidentate series. Ongoing computational studies and cyclic voltammetry aim to establish structure–electronic property relationships, and initial findings suggest that these complexes may interact with biologically relevant targets. These results provide insight into how NS ligand hapticity and phosphine substitution modulate electronic properties and reactivity, with potential implications for catalytic and metallodrug applications.



Synthetic route to [Ru(η6-p-cymene)(κS-MCBTZ)(PR3)Cl]PF6 and [Ru(η6-p-cymene)(κ2N,S-MCBTZ)(PR3)]BF4

Agradecimentos/Acknowledgments

I acknowledge the Federal University of Santa Catarina (UFSC) for institutional support and the CNPq for essential funding. I also thank the Medicinal Inorganic Synthesis and Catalysis Group (GSIMC) for guidance.

Elucidação estrutural de um ligante tripodal inédito e seu complexo mononuclear de cobre(II) por DRX e XAS

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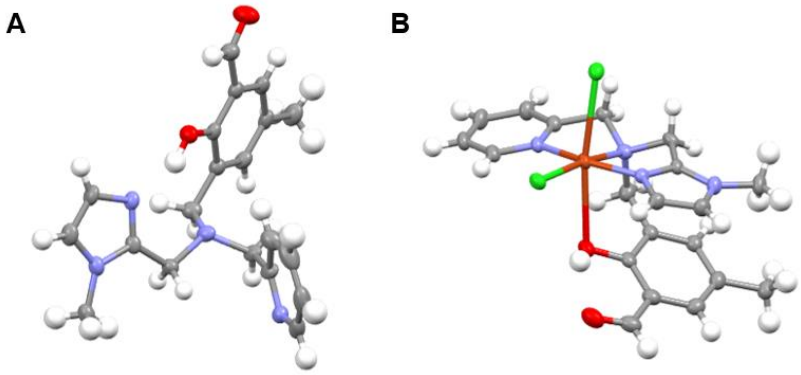
Palavras Chave:*Ligantes tripodais,complexo de cobre(II),caracterização estrutural,DRX,XAS*

Highlights

Novo ligante e complexo de Cu 2+ foram estudados por absorção e difração de raios X, assim como outras espectroscopias clássicas, permitindo a elucidação inequívoca de suas propriedades estruturais.

Resumo/Abstract

Ligantes tripodais constituem uma classe versátil de moléculas caracterizadas por um átomo central que organiza três braços coordenantes, capazes de interagir simultaneamente com diferentes regiões de um alvo biológico ou um centro metálico [1]. A alta flexibilidade conformacional, facilidade de ajuste estérico e densidade eletrônica distribuída conferem propriedades particularmente atrativas para aplicações medicinal-inorgânicas. Neste contexto, um ligante tripodal inédito, X1PMAMFF, foi sintetizado, juntamente com seu respectivo complexo mononuclear de cobre(II) (Figura 1), e ambos foram completamente caracterizados em solução e no estado sólido. O ligante é composto por três substituintes aromáticos: uma piridina, um anel metilimidazólico e um anel metil-formilfenólico. A difração de raios X por monocristal mostrou que X1PMAMFF apresenta uma desordem conformacional nos anéis nitrogenados, tendo a posição preferencial 75% de ocupação. Já o complexo tem seu arranjo preferencial com 85% de ocupação, mantendo uma desordem similar à do ligante. A esfera de coordenação foi determinada por espectroscopia de absorção de raios X, que indicou uma coordenação do tipo 3N2ClO, com valores médios de distâncias de ligação de 1,97 ± 0,02 Å (nitrogênios), 2,22 ± 0,03 Å (cloretos) e ~2,8 Å (oxigênio). Pela DRX foi possível confirmar que o íon cobre(II) adota uma geometria octaédrica distorcida, com contatos axiais envolvendo o fenol e um dos íons cloreto, a uma distância maior devido ao efeito Jahn-Teller. A determinação inequívoca da esfera de coordenação de um complexo inédito é fundamental para o estudo de sua atividade farmacológica e/ou catalítica. Espera-se que a presença de dois sítios lábeis seja capaz de conferir ao complexo a capacidade de ligar-se a biomoléculas de interesse como o DNA no âmbito do câncer e determinadas proteínas no contexto de doenças neurodegenerativas, o que será avaliado em trabalhos futuros.
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Representação ORTEP das estruturas de (A) X1PMAMFF e (B) seu complexo de cobre(II), medidas por DRX.

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PIBIC UERJ, FAPERJ, CNPq, LNLS

Engineering Spinel and Heterostructured Oxides from MOFs for High-Performance Oxygen Evolution

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Palavras Chave:*OER,Electrocatalysis,MOF,MOF-Derived,Water splitting,OER,MOF,MOF-derived,Electrocatalysis,Hydrogen*

Highlights

MOF-Derived spinel oxides achieve competitive OER performance among non-nobel metal electrocatalysts. Tailored MOF precursors drive synergic effects and improved OER kinetics in mixed-metal oxides

Resumo/Abstract

Metal–organic frameworks (MOFs) and coordination polymers have become strategic precursors for the design of advanced metal-oxide electrocatalysts for the oxygen evolution reaction (OER). Since 2021, the SIAP research group at the Federal University of Paraíba (UFPB) has established a systematic research line in the Brazilian Northeast focused on MOF-derived mono-, bi- and heterometallic oxides and spinels for alkaline OER. Using MOFs as structural and chemical templates, our studies demonstrate precise control over composition, mixed-valence states, porosity and heterointerfaces, leading to enhanced intrinsic activity and reaction kinetics. MOF-templated manganese–cobaltites, nickel–cobaltites and ferrites exhibit low overpotentials at 10 mA cm^{-2} (typically below ~350 mV) and favorable Tafel slopes frequently below ~70 mV dec^{-1}, highlighting the synergistic effects between mixed-metal centers and defect-rich oxide frameworks. MOF-derived heterostructures such as CeO_2/Co_3O_4, CuO/Cu_2O and Cu–Co oxides further show improved charge-transfer properties, high electrochemically active surface areas and long-term stability under continuous polarization. Recent advances involving metal-ion impregnation in ZIFs and MOF-on-MOF architectures enable the formation of highly active spinel phases (e.g., MCo_2O_4 and $CuCo_2O_4$), delivering competitive OER performance comparable to state-of-the-art non-noble metal catalysts, while also allowing bifunctional behavior toward energy storage applications. Collectively, these results consolidate the Brazillian research on MOF-derived metal oxides as a robust and versatile platform for OER electrocatalysis for green hydrogen technologies.

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Entrega seletiva de complexos de ouro(III) em células tumorais a partir de lipossomas contendo porfirazina de Mg(II).

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Palavras Chave:*Câncer,Porfirazina,Complexo de ouro(III).*

Highlights

The use of a porphyrazine to promote drug release is unprecedented and has potencial to destroy tumor cells selectively.

Resumo/Abstract

A internalização fotoquímica (PCI) é uma técnica que utiliza um fotossensibilizador e luz para a entrega de moléculas terapêuticas em células-alvo, visando maximizar a eficiência do tratamento e reduzir efeitos adversos [1]. Assim, sabendo que um complexo de ouro(III) derivado de tiocarbamato (C3b) possui alta toxicidade, porém baixa seletividade para células de câncer de mama triplo-negativo (MDA-MB-231) [2], o objetivo deste trabalho é investigar o potencial de associação de um fotossensibilizador, a porfirazina de magnésio(II) (MgPz), junto ao complexo C3b em sistemas lipossomais para aprimorar a seletividade tumoral e a sua eficiência terapêutica. As formulações contendo apenas MgPz, a combinação (MgPz+C3b) e apenas C3b foram preparadas pelo método de hidratação do filme lipídico seguido de extrusão em membranas de 100 nm [3]. Após a purificação em coluna de Sephadex, obteve-se uma taxa de encapsulamento de 70,9% para o complexo de ouro(III). A atividade fototerapêutica foi realizada em linhagens celulares de carcinoma de células escamosas (A431), comparando-se grupos mantidos no escuro e grupos irradiados com LEDs vermelhos (620-630 nm) por 30 minutos. Os ensaios de viabilidade revelaram que a citotoxicidade moderada do C3b não foi influenciada pela luz, contudo, a formulação completa (MgPz+C3b) exibiu um aumento da toxicidade no escuro, que se potencializou ainda mais sob luz. Como resultados análogos foram observados para os lipossomas contendo apenas MgPz, conclui-se que a toxicidade predominante é originada majoritariamente da porfirazina. Logo, estudos futuros devem se concentrar na otimização das formulações para encontrar a concentração ideal de porfirazina que atue como um ativador eficiente da liberação intracelular de C3b e, assim, potencialize a ação desejada deste como agente terapêutico. [1] JERJES, W et al. J. Clin. Med. 9, 2020, 528. [2] QUERINO, A. L. A et al. J. Inorg. Biochem. 247, 2023. [3] PINHEIRO, A. P. et al. Photochem. Photobiol. Sci. 23, 2024.

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Estudo à obtenção de compostos de Terra Rara com Macrocíclicos: Projeção de compostos fotossensíveis com potencial aplicação biomédica

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Palavras Chave:*Lantanídeos,fotossensível,biomedicina,macrocíclicos,terras raras*

Highlights

Developing photosensitive lanthanide complexes with macrocyclic ligands: a comparative study of synthetic routes for advanced biomedical applications.
Lanthanide-cyclam: a comparative study.

Resumo/Abstract

Íons trivalentes de Terra Rara (TR) ou Lantanídeos são metais de transição interna que, por apresentarem propriedades ópticas e magnéticas únicas, possuem uma gama de aplicações, como na indústria de materiais magnéticos, na óptica a laser, em sondas luminescentes, na terapia fotodinâmica contra o câncer e na fixação a biomoléculas. Esses metais possuem baixos coeficientes de absorção e, por esse motivo, em algumas aplicações, são utilizados ligantes cromóforos que agem como uma “antena”, transferindo a energia incidida sobre o complexo, para o centro metálico. Somado a isso, ligantes como os macrocíclicos derivados do Cyclam auxiliam o metal em algumas interações biológicas, por proporcionar estabilidade termodinâmica e cinética ao centro metálico dentro do corpo humano. Com isso, a união desses íons a matrizes macrocíclicas tem sido utilizada em diversas áreas da ciência para maximizar e moldar tais propriedades. Portanto, o presente trabalho trata-se de um estudo teórico e experimental que tem como objetivo refinar métodos de obtenção de complexos de TR(III) nos quais seja possível formulá-los para que apresentem atividade fotossensível e biológica através deste design. Com isso, foi realizada uma revisão bibliográfica utilizando o portal de periódicos da Capes para a coleta de artigos publicados a partir dos anos 2000, de grupos de pesquisas consolidados e alinhados com o interesse desta pesquisa. Para tanto, está sendo realizado um estudo comparativo entre duas rotas de síntese utilizando diferentes sais de TR, a fim de determinar a metodologia mais adequada, a qual servirá de modelo para as sínteses. O estudo e as caracterizações se encontram em andamento; porém, até o presente momento, caracterizações como RMN de ^{1}H, RMN de 13C, espectroscopia no infravermelho e análise elementar mostraram que a coordenação entre os ligantes e o centro metálico ocorreu, comparativamente com êxito, em todas as síntese realizadas, partindo dos sais de nitratos.

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Evaluating docking software performance for the formate-heme interaction

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Palavras Chave:*Docking,Computational chemistry,Force field,Metalloprotein*

Highlights

Analysing docking sotware accuracy for metal-ligand systems, this study compares simulated Fe-O bond lengths in formate-heme complexes against crystallographic data to validate force field parameters.

Resumo/Abstract

The computational analysis of ligand-protein interactions is fundamental to bioinorganic chemistry, particularly within the framework of drug design. Docking software packages facilitate initial screening phases by providing high-throughput, cost-effective simulations that elucidate ligand-binding site interactions. These techniques typically employ certain simplifications, such as the utilization of rigid protein backbones and the substitution of high-level quantum mechanical calculations with force field approximations [1]. However, many software lack the ability to simulate interactions involving metallic atoms [2]. Consequently, validating a software's parameters for a specific ligand-protein system is essential for ensuring the reliability of the results. This study evaluates several widely utilized docking programs to characterize the interaction between formate and the heme group, specifically assessing whether the underlying force fields provide an accurate Fe–O interaction parameter. Accuracy is determined by comparing the Fe–O bond length of the optimal binding pose [2] against experimental crystallographic data for this complex [3].

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Fast Naproxen Removal Catalyzed by Mn–Porphyrin and Oxone®: Performance, Mechanism, and Toxicity

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Palavras Chave:*Catalyst,Metalloporphyrins,Environment,Oxone,EPR*

Highlights

Scienciometric analysis of naproxen degradation, experimental to optimized Mn-porphyrin/Oxone® catalytic systems, and active species ($O_2{\cdot}^-$ and $^1O_2$) identified via scavengers and EPR.

Resumo/Abstract

As a nonsteroidal anti-inflammatory drugs, naproxen is an emerging pollutant frequently detected in surface and wastewater. In the environment, it may cause harmful effects including mutagenic alterations in bacterial systems, teratogenic effects in aquatic organisms, and the proliferation of antibiotic-resistant bacteria in humans [1]. In this study, two manganese porphyrins — chlorido-5,10,15,20-tetrakis(4-carboxyphenyl)porphyrinatemanganese(III) [Mn(T4CPP)Cl] (**MnP1**) and chlorido-5,10,15,20-tetrakis(4-trimethylammonium)porphyrinatomanganese(III) [Mn(T4MAPP)]Cl_5 (**MnP2**) — were evaluated as catalysts with Oxone® to degrade naproxen. Experimental conditions were investigated using a central composite design for each catalyst. Molar ratios of catalyst:naproxen:Oxone® tested were 1:10:50, 1:10:125, 1:10:200, 1:10:19, and 1:10:230, with reaction times of 30, 75, 120, 11, and 140 minutes. For**MnP1**, no suitable model was obtained because responses did not vary within the experimental ranges. In contrast, whit**MnP2**, up to 87% naproxen degradation was achieved in 30 minutes at a**MnP2**:naproxen:Oxone® ratio of 1:10:50. The formation of reactive species was investigated using radical inhibitors and electron paramagnetic resonance (EPR) with spin traps [2], detecting superoxide radical ($O_2{\cdot}^-$) and oxygen singlet ($^1O_2$). The germination assays (Lactuca sativa), applied to analyze phytotoxicity, indicated the studied system (30 minutes at a**MnP2**:naproxen:Oxone® ratio of 1:10:50) phytotoxic; whereas**MnP2**alone showed no phytotoxicity. Future studies will target milder reaction conditions to maximize naproxen degradation and reduce the phytotoxicity.

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[2] H.F.V. Victória et al., Free Radic. Biol. Med. 180 (2022) 143–152. https://doi.org/10.1016/j.freeradbiomed.2021.12.303.

Agradecimentos/Acknowledgments

CAPES, CNPq, INCT-CiMol, FAPEMIG, (FINEP), LAREMAR, CEI-DQ/UFMG, NEPS-DQ, PRPQ/UFMG.

From ink to stamp: multifunctional luminescent platforms for anti-counterfeiting

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Palavras Chave:*Polyvinyl alcohol,Luminescent stamp,Printing technique*

Highlights

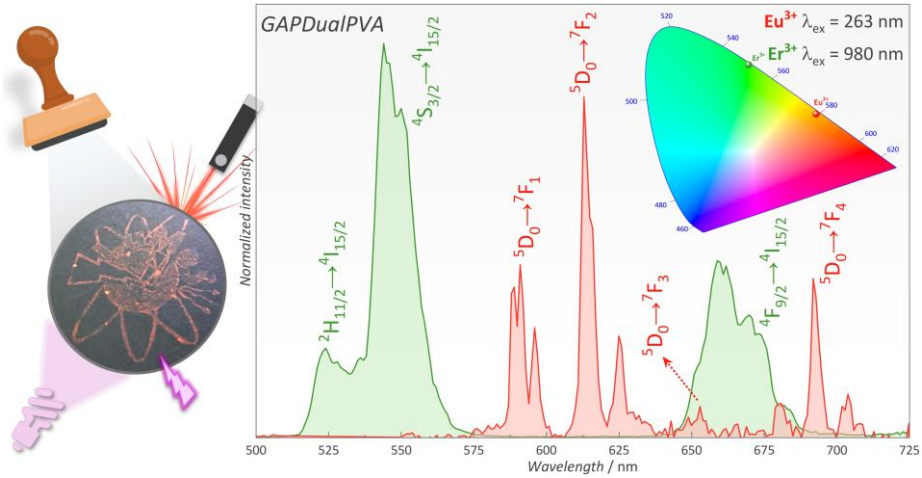
$GdAlO_3:Eu^{3+}$ and $GdAlO_3:Er^{3+},Yb^{3+}$ phosphors via urea combustion method. PVA-based ink with downshifting and upconversion luminescence. Dual-excitation layer luminescent stamp for anti-counterfeiting.

Resumo/Abstract

Counterfeiting of banknotes, jewelry, art, documents, and pharmaceuticals is a growing global issue affecting the economy, security, and health. Therefore, flexible, non-toxic, low-cost anti-counterfeiting techniques using rare-earth ion-based (RE^{3+}) multifunctional luminescent inks have been developed as an effective alternative for security applications, resulting in a material with combined inorganic-organic properties[1]. This study reports photoluminescent stamps with dual UV and IR excitation layers, fabricated from polyvinyl alcohol (PVA) ink containing $Gd_{0.97}AlO_3:Eu^{3+}{}_{0.03}$ (downshifting – DS) and $Gd_{0.96}AlO_3:Er^{3+}{}_{0.01},Yb^{3+}{}_{0.03}$ (upconversion - UC) phosphors. This multifunctional ink was made using both phosphors synthesized via urea combustion method[2], 10% (w/w) PVA solution, ethanol, water, glycerol, and Triton X-100. Luminescent stamp patterns were applied to banknotes and black paper. XRD patterns and Rietveld refinement confirm that DS and UC phosphors form the target orthorhombic perovskite phase (*Pbnm*space group). Ink stability in suspension, assessed via zeta potential (ZP) (pH 3.80-9.75, 4 to -6 mV with an isoelectric point,*IEP,*of 5.60) and DLS (polydispersity index,*PdI,*of 0.572) data indicates limited polymer-phosphor interaction but sufficient dispersion for stamping. The ink exhibits dual emission: red (Eu^{3+}, 95.1% purity at 263 nm excitation) and green (Er^{3+}, 97.1% purity at 980 nm excitation). Kinetic measurements monitoring UC transitions showed lifetimes of 0.15-0.19 ms, while DS monitoring the 0-1, 0-2, and 0-4 transitions of Eu^{3+} yielded in 1.46-1.77 ms. The stamped ink on various substrates displays visible dual emission under different excitation, supporting its anti-counterfeiting application.

[1]H. Jia,*et al.*, ACS Materials Lett. 2022, 4, 1306−1313.

[2] P. Kumar,*et al.*, Inorg. Chem. Commun. 2022, 145, 110064.



Downshifting and upconversion emission spectra for the dual luminescent ink applied to the stamp.

Agradecimentos/Acknowledgments

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Frontiers of Innovation in Inorganic Chemistry: Emerging Trends and Technological Drivers

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Palavras Chave:*Inorganic Chemistry, Technological Forecasting, Patentometry, Intellectual Property, Patents*

Highlights

Patent landscape in inorganic chemistry was built.

High-quality patents highlight advances in electrochemical energy storage, light-metal rechargeable systems, and carbon Si advanced materials.

Resumo/Abstract

A patent search was conducted on the Lens platform focusing on patents classified within the field of inorganic chemistry. For this purpose, the search strategy shown in Figure 1 was employed.

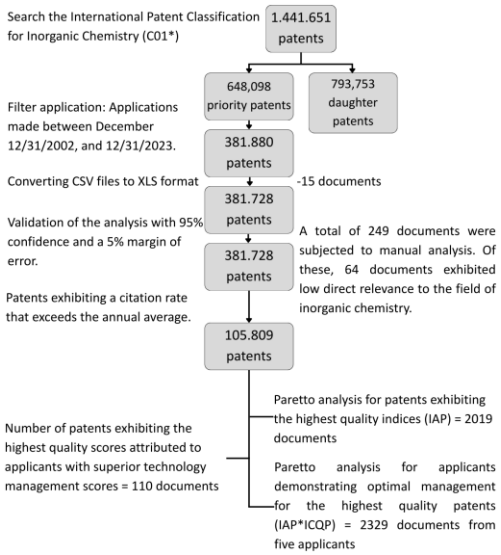
The quality indicators used in this study include variables such as: GII; applied patents; patent families; domestic to foreign patent applications; average patent citation rate; maintenance rate; success rate in the conversion of applications into granted patents.

Of the 2,019 documents analyzed, 46% remain active and 37% are no longer valid. The ranking of countries with the highest number of patent filings differs from that observed when considering the countries holding patents with the highest quality indices.

The group of applicants responsible for the highest-quality patents is composed exclusively by companies, in contrast to the group of the largest applicants by volume, in which Chinese universities stand out as the most active applicants.

The analysis of the technical descriptions of the patents reveals a central domain structured around electrochemical energy storage focusing on rechargeable systems based on the insertion and intercalation of light metals. Li-ion batteries including alternative systems based on Mg and Al, supported by the mixed oxides and transition-metal hydroxides, as well as carbon-based materials, and Si. The relevance of microstructural control, nanotechnology, and the systematic use of advanced structural and microscopic characterization techniques is also evident, together with the incorporation of recycling, materials recovery, catalytic processes, H_2, CO_2 and circular economy strategies.

Overall, the analyzed documents exhibit a profile of predominantly incremental innovation, based on technical refinements, with the identification of opportunities for further development and potential technology transfer. This set of elements contributes significantly to prospecting future innovations.



Workflow for Selecting High-Quality Patent Documents for Analysis

Agradecimentos/Acknowledgments

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Funcionalized silica as a platform for Ir3+ and Eu3+ based luminescente hybrid

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Palavras Chave:*iridium, europium , sol-gel method, silica particles, surface modification.*

Highlights

Luminescent hybrid with emission in the yellow and red regions based Ir^{3+} and Eu^{3+} complexes anchored to the silica surface.

Resumo/Abstract

The anchoring of luminescent species in stable and biocompatible matrices has become an important topic of scientific research because it enables the development of new advanced optical systems[[i]]. These systems combine adjustable photophysical properties with the mechanical, morphological, and chemical characteristics of the host material. As a result, functional platforms have high potential for biological and technological applications[[ii]]. In this context, the combination of functionalized silica particles capable of anchoring lanthanide ion complexes and Ir^{3+} complexes become a promissing strategy for obtaining efficient and low-toxic luminescent stain[[iii]].and based on Scanning Electron Microscopy (SEM) analysis, an average diameter of 254 nm was estimated. From these particles, two luminescent hybrid were obtained. The hybrid containing the iridium complex, [Ir(fppy)(bqdc-Si_2)]-SiO_2,when excited at 320 nm, emits from the MLCT state, this hybrid showed a maximum emission at 590 nm, in the yellow region and color purity of 73%. The Absolute quantum yield determined for the powder of this hybrid was 0.85%. Similarly, for the hybrid [$Eu(tta)_3$(bqdc-Si_2)]-SiO_2 excited at 393 nm, a maximum emission at 614 nm was observed, attributed to the hypersensitive transition $^5D_0 \rightarrow {}^7F_2$ of the Eu^{3+}ion, exhibiting an emission in the red region with a color purity value of 74%. For this material, an absolute quantum yield value of 2.3% was determined. Thus, the joint analysis of the luminescent, structural, and morphological properties indicates that the hybrid has potential for application in bioimaging.

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[ii]WU, D. et al. Fluorescent chemosensors: the past, present and future. Chemical Society Reviews, v. 46, n. 23, p. 7105-7123, 2017.

[iii] SANTOS, J. A. O et al. Red-emitting hybrid based on eu3+-dbm complex anchored on silica nanoparticles surface by carboxylic acid for biomarker application. Materials, v. 13, n. 23, p. 5494, 2020.

Agradecimentos/Acknowledgments

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Gold complexes with NHC and phosphine ligands as therapeutic candidates for Leishmaniasis: experimental and computational studies.

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Palavras Chave:*Leishmaniasis,Gold Complexes,N-Heterocyclic Carbene,DFT.*

Highlights

Gold complexes as potential antileishmanial agents.

NHC ligand precursor synthesized and characterized by ^{1}H NMR.

DFT calculations link lower HOMO-LUMO gaps to higher cysteine and aquation reactivity.

Resumo/Abstract

Leishmaniases are a group of neglected tropical parasitic diseases[1]. Current treatments for these diseases present several drawbacks, including high toxicity, administration routes unsuitable for treatment, and high associated costs. Our group investigates new therapies for leishmaniases based on gold complexes, with some of them showing promising results ([Au(IMes)Cl] and [Au(IBn)Cl] presenting EC_{50}values of (1.57 ± 0.41) and (1.65 ± 0.16) μM with Selectivity Index of 13.9 and 11.2, respectively, against L. amazonensis)[2]. Gold complexes act against these diseases mainly due to their thiophilicity and the presence of thiol and selenol groups in the active sites of trypanothione reductase (TR).

In this work, the in vitro antileishmanial activities of a systematic series of six gold complexes bearing an NHC ligand and p-(COOHPh)Ph_2P are evaluated and correlated with experimental and computational studies (Figure 1).

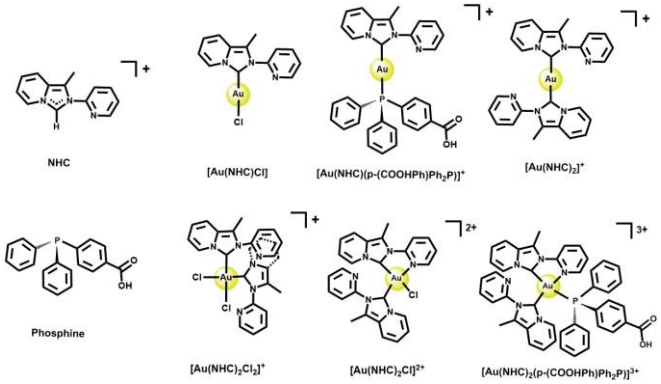
The precursor structure of the ligand employed was successfully synthesized and characterized by ^{1}H NMR[3]. Density Functional Theory (DFT) studies, performed using the ORCA package version 6.0 employing PBE0 functional, SARC-ZORA-TZVP and ZORA-def2-TZVP basis sets and CPCM model for DMSO implicit solvation, indicate that the direct reaction of the complexes with cysteine is more favorable than reaction via an aquation intermediate, due to the high ΔrG° value of the aquation intermediate formation reaction. DFT studies also indicate that lower HOMO–LUMO gaps are associated with higher reactivity of the complexes toward cysteine. The complex $[Au(NHC)_2Cl]^{2+}$, which exhibits the lowest gap (3.54 eV), showed the highest reactivity toward cysteine, with a ΔrG° of 4.0 kcal.mol^{-1}, whereas [Au(NHC)Cl], which has the highest gap (4.35 eV), showed the lowest reactivity, with a ΔrG° of 9.5 kcal.mol^{-1}.

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Ligands and gold complexes investigated in this work.

Agradecimentos/Acknowledgments

This work was carried out with support from the São Paulo Research Foundation (FAPESP), Brazil. Process No. 2025/12452-0.

GOLD(I)–NHC COMPLEXES CONTAINING SELENIUM AS POTENTIAL THERAPEUTIC ALTERNATIVES FOR LEISHMANIASIS

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Palavras Chave:*Leishmaniasis, Gold(I), N-heterocyclic carbenes, Selenium, Organometallics,Leishmaniasis,Gold(I),N-heterocyclic carbene,Selenium,Organometallic*

Highlights

Gold(I)–NHC complexes containing selenium show high and selective anti-Leishmania activity at low micromolar concentrations, highlighting their potential as innovative therapeutic candidates.

Resumo/Abstract

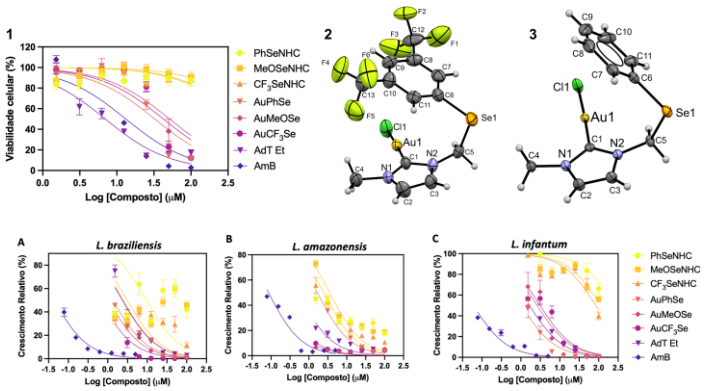
Leishmaniases constitute a group of neglected tropical diseases caused by protozoa of the genus*Leishmania*and are associated with high morbidity and mortality. Despite their substantial epidemiological impact, the currently available therapeutic arsenal remains limited, being characterized by significant toxicity, parasite resistance, and administration constraints, which underscores the need for more effective and safer therapeutic alternatives.

In this context, gold-based metal complexes have emerged as promising candidates, particularly due to their high chemical stability and well-documented biological activity. Gold(I) complexes bearing N-heterocyclic carbene (NHC) ligands are distinguished by their chemical robustness, while the incorporation of the calcogen element selenium is especially attractive owing to its close association with cellular redox processes. Such processes are critical for the survival of*Leishmania*parasites, whose redox homeostasis is predominantly regulated by the trypanothione system.

Herein, we report the synthesis of selenium-containing gold(I)–NHC complexes via a transmetallation route using Ag_2O as the carbene-generating agent, under an inert N_2 or argon atmosphere, with reactions conducted overnight. Single crystals suitable for structural analysis were obtained by slow diffusion in ether. The complexes were thoroughly characterized by infrared spectroscopy, UV–Vis, fluorescence spectroscopy, ^1H and ^13C NMR, mass spectrometry, CHN elemental analysis, and single-crystal X-ray diffraction.

Biological activity was assessed through cytotoxicity assays in human macrophages derived from the THP-1 cell line and anti-amastigote assays against*Leishmania braziliensis*,*L. amazonensis*, and*L. infantum*, employing genetically modified parasites expressing luciferase as a reporter gene. The complexes exhibited pronounced antileishmanial activity at low micromolar concentrations (< 2 µM), combined with high selectivity toward human macrophages. Notably, the AuMeOSe complex displayed an IC_{50} value of 0.2 µM and a selectivity index of 255 against*L. amazonensis*. Preliminary interaction studies with glutathione (GSH) were conducted as an initial step toward future investigations involving parasite redox enzymes.

The innovation associated with these systems supported the filing of a patent application and is corroborated by the results, which highlight their potential as promising candidates for the development of new antileishmanial therapies.



Cytotoxicity in THP-1 cells, AuNHC and AuCF3 crystal structures, and anti-Leishmania activity.

Agradecimentos/Acknowledgments

FAPEMIG, CNPq, CAPES, Departamento de Química da UFMG e Instituto René Rachou–Fiocruz Minas.

Heteroleptic Nickel(II) complexes with aromatic and aliphatic ligands: A theoretical-experimental electronic investigation

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Palavras Chave:*Xanthate,Nickel(II),Infrared,Crystal structure,TD-DFT.*

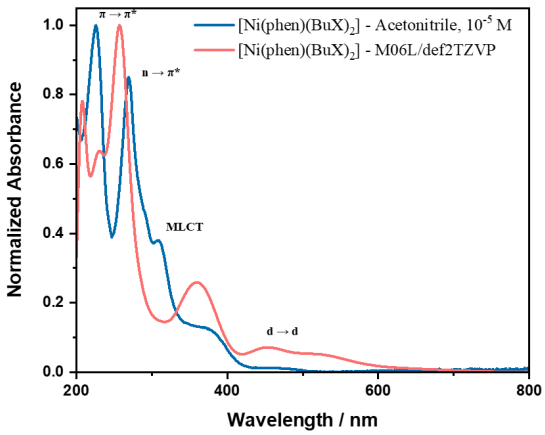
Highlights

Three heteroleptic Ni(II) complexes containing xanthate and 1,10-phenanthroline ligands were synthesized and characterized by spectroscopic theoretical-experimental analyses.

Resumo/Abstract

Due to their properties, heteroleptic nickel(II) complexes exhibit biological activities, such as antibacterial effects[1]. In this work, three heteroleptic nickel(II) complexes were synthesized and characterized:**[Ni(phen)(PrX)$_2$]**,**[Ni(phen)(^{i}PrX)$_2$]**, and**[Ni(phen)(BuX)$_2$]**, according to procedures described in the literature[2]. The previously synthesized ligands (*n*-propyl (PrX),*iso*-propyl (^{i}PrX), and*n*-butyl (BuX)) were characterized by infrared spectroscopy, Raman scattering, and UV-Vis spectroscopy (acetonitrile, 10^{-3} and 10^{-5} M). The vibrational spectra of the complexes exhibited bands around 1240, 1100, 1048, and 675 cm^{-1}, and 1030, 660, 465, and 385 cm^{-1}, corresponding to the vibrational modes υ_{as}(C-O-C), υ(C=S), υ_s(C-O-C), υ(C-S), and υ_{as}(S-C-S), υ(C=S), δ_{as}(C-O-C), for infrared and Raman scattering, respectively. The UV-Vis solution spectra showed the presence of intraligand electronic transitions involving both the xanthate and 1,10-phenanthroline (phen) ligands. In addition to these transitions, metal to ligand charge transfer (MLCT) and d-d electronic transitions were also identified. Single crystals of the complex containing the BuX ligand were obtained, which exhibited a crystalline structure with the formula [Ni(phen)(BuX)$_2$], featuring a distorted octahedral geometry, with two xanthate ligands and one phenanthroline ligand coordinated in a bidentate fashion to the metal center. In addition, TD-DFT and natural bond orbital (NBO) analyses were performed, comparing heteroleptic and analogous homoleptic xanthate complexes. The results confirmed all the electronic transitions involved in the xanthate and phen ligands, as well as the transitions from the metal center (Figure 1). All calculations employed the DFT/M06L/def2-TZVP level of theory using Gaussian 09 and GaussSum.

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[2] Johnson A.L.; et al. Inorganic Chemistry Communications 2014, 49, 8-11.



Theoretical-experimental comparison of the UV-Vis spectrum of the complex [Ni(phen)(BuX)2].

Agradecimentos/Acknowledgments

CNPq, CAPES, FAPERJ, LDRX, LMQC, LAME and PROPPi

Highly Selective Pd(II) Thiosemicarbazone Complexes with Potent Cytotoxic Activity against Ovarian Cancer Cells.

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Palavras Chave:*Palladium complexes;,Thiosemicarbazones;,Ovarian Cancer;,Selectivity Index*

Highlights

Four novel Pd(II)–thiosemicarbazone complexes were synthesized and fully characterize. The high selectivity index (SI = 312) highlights the potential of these complexes as antitumor candidates.

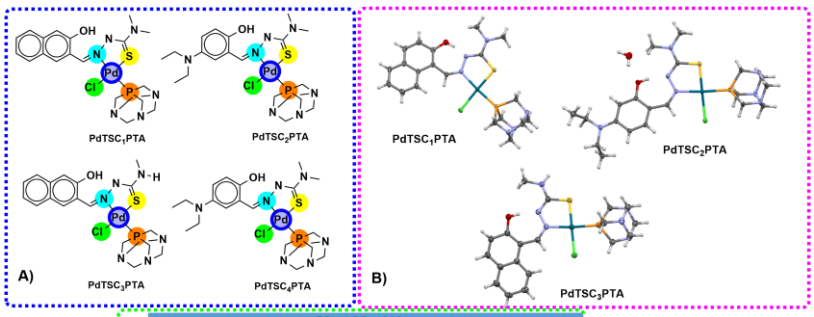
Resumo/Abstract

Cancer is a highly heterogeneous group of diseases and remains a major global health challenge, with 19.3 million new cases reported in 2020 and an estimated lifetime risk of one in five individuals[1]. In this context, the development of new therapeutic agents with improved efficacy and selectivity is essential. Although metal-based drugs have long been explored in medicine, their clinical application is often limited by severe side effects, as exemplified by cisplatin, which lacks tumor selectivity[2]. In this work, novel PdII-based complexes were developed aiming to combine high cytotoxic activity with enhanced selectivity. Four new palladium(II) complexes with the general formula [Pd(TSC_1–$_4$)(PTA)Cl], where TSC_1–$_4$ are thiosemicarbazone ligands and PTA is 1,3,5-triaza-7-phosphaadamantane, were synthesized and characterized by IR, NMR, and X-ray diffraction, confirming coordination through nitrogen and sulfur atoms. Biological assays against tumor (A2780, ovarian cancer) and non-tumor (MRC-5, lung fibroblast) cell lines revealed that PdTSC4PTA exhibits potent cytotoxicity toward A2780 cells (IC_{50} = 0.16 μM) while showing no toxicity toward healthy cells up to 50 μM, resulting in a high selectivity index of 312. These results highlight the promising antitumor potential of these Pd(II) complexes.

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(2) Anthony, E. J.; Bolitho, E. M.; Bridgewater, H. E.; Carter, O. W. L.; Donnelly, J. M.; Imberti, C.; Lant, E. C.; Lermyte, F.; Needham, R. J.; Palau, M.; Sadler, P. J.; Shi, H.; Wang, F. X.; Zhang, W. Y.; Zhang, Z. Metallodrugs Are Unique: Opportunities and Challenges of Discovery and Development.*Chem. Sci.***2020**,*11*(48), 12888–12917. https://doi.org/10.1039/d0sc04082g.



C)

IC50 (μM) – 24 hrs					
Complexes	MRC-5	A2780	A2780cis	IS*	IS**
PdTSC1PTA	3.37 ± 0.310	0.230 ± 0.0500	1.22 ± 0.250	14.6	2.76
PdTSC2PTA	4.20 ± 0.300	0.360 ± 0.0200	1.94 ± 0.110	11.7	2.16
PdTSC3PTA	5.49 ± 0.960	0.260 ± 0.0500	0.770 ± 0.0600	21.1	7.13
PdTSC4PTA	>50.0	0.160 ± 0.0100	-	312	-
Cisplatin	12.5 ± 0.150	11.2 ± 0.300	25.6 ± 0.290	1.11	0.488

Figure 1. A) Palladium complexes. B) Crystallographic structures. C) IC50 table for the complexes.

Agradecimentos/Acknowledgments

FAPESP (2025/14380-7 and 2025/07533-1)and CNPq (305259/2025-3)

Hydrometallurgical routes for recovering rare earth oxides from fluorescent lamps recycling waste for the production of functional materials

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Palavras Chave:*Rare earths,Urban mining*

Highlights

Combined acid leaching, oxalate precipitation and alkaline fusion strategies enable efficient recovery of phase-pure Y/Eu and Tb/La/Ce-rich oxides from fluorescent lamp waste.

Resumo/Abstract

The increasing demand for rare earth elements and the environmental impacts associated with primary mining have stimulated the development of alternative recovery routes from secondary sources. In this study, different routes were investigated to recover rare-earth oxides from industrial fluorescent lamp recycling waste, focusing on impurity removal and the production of materials suitable as precursors for functional photonic applications. Fluorescent lamp powders (<38 µm) were subjected to acid leaching with HCl or H_2SO_4 aqueous solutions for 24 h, with and without an acid pre-treatment consisting of a 30 min leaching step to remove calcium-based impurities. The resulting leachates were precipitated with oxalic acid to form Y and Eu oxalates, followed by calcination at 800 °C to obtain the corresponding oxides. The effects of acid type, temperature, and pH control on precipitation efficiency were evaluated. In a subsequent step, the solid residues were treated by alkaline fusion with NaOH, followed by calcination, acid leaching, and oxalic acid precipitation, aiming at the additional recovery of rare earths not initially leached, including Tb, La, and Ce. The recovered materials and solid wastes were characterized by powder X-ray diffraction (XRD) and energy-dispersive spectroscopy (EDS) and photoluminescence spectroscopy (PL). Acid pre-treatment was critical to obtain phase-pure Y_2O_3:Eu^{3+} via the HCl route, whereas H_2SO_4 enabled similar phase purity without pre-treatment due to $CaSO_4$ formation during leaching. The alkaline fusion route proved effective for recovering a Tb/Ce/La-rich oxide from HCl-leached residues. Overall, the combined use of controlled acid leaching, oxalate precipitation, and alkaline fusion represents a promising strategy for rare-earth recovery from fluorescent lamp waste, contributing to waste valorization and resource reuse.

Agradecimentos/Acknowledgments

Authors thank CNPq (grant 407747/2022-2) and FAPESP (grant 2025/08960-0) for financial support.

Hydroxyl radical generation and x-ray–mediated apoptosis induction in human breast cancer cells treated with Ruthenium-Phthalocyanine complexes

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Palavras Chave:*Ruthenium-phthalocyanine complexes,Radiodynamic therapy,Breast cancer cells,Apoptosis*

Highlights

Ruthenium–phthalocyanine complexes generate hydroxyl radicals upon X-ray irradiation, enabling radiodynamic therapy.

Resumo/Abstract

Photodynamic therapy is a promising alternative based on photosensitizer activation by visible light; however, limited tissue penetration and skin phototoxicity restrict its use. Radiodynamic therapy (RDT) emerges as an alternative [1]. This study investigated RDT using the complexes $(^{n}Bu_4N)_2$ $[RuPc(NO_2)_2]$ (Complex I) and*trans*-[Ru(NO)Pc(ONO)] (Complex II) in human breast cancer MCF-7 cells. To investigate whether the complexes produce reactive oxygen species, hydroxyl radical detection assays were performed using fluorescence techniques. Both complexes generate hydroxyl radicals when exposed to X-ray radiation. Cell viability was assessed by the MTT assay and both complexes exhibited cytotoxicity only under X-ray irradiation, while no cytotoxic effects were observed without irradiation. Long-term effects were evaluated by the clonogenic assay, in which both complexes inhibited colony formation at 10 µM under X-ray irradiation. The effects on the cytoskeleton and cell proliferation were evaluated by immunofluorescence. Treatment with 5 µM combined with X-ray irradiation caused marked cellular disorganization and inhibition of proliferation, evidenced by the absence of Ki-67 expression. Apoptotic effects were further investigated by nuclear fragmentation assays, flow cytometry, and PARP Western blotting. Both complexes induced pronounced nuclear fragmentation at 5 µM following X-ray irradiation, characterized by nuclear disintegration, indicating activation of apoptotic pathways. Annexin V/flow cytometry analysis revealed predominant late apoptosis after 24 h, associated with loss of membrane integrity. Western blotting analysis confirmed PARP cleavage, indicating caspase-3-mediated apoptosis. Further studies using three-dimensional tumor models and normal cells will be conducted to better evaluate therapeutic efficacy and safety under conditions closer to in vivo systems.
[1] Zhu S, et al. Theranostics. 2023;13(3):1042-1058. doi:10.7150/thno.78649.

Agradecimentos/Acknowledgments

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Impact of High-Energy Radiation on the Photostability of Lanthanide β-Diketonate Complexes

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Palavras Chave:*Lanthanide complexes,Photostability,Luminescence*

Highlights

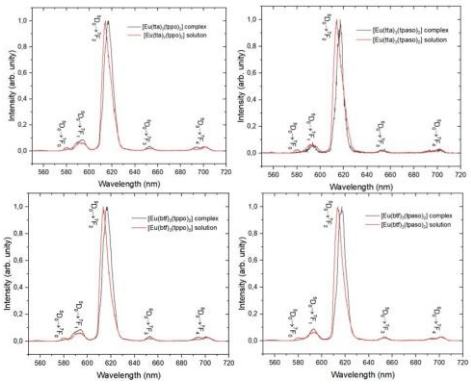
Investigation of trivalent europium complexes photodegradation, coordinated to β-diketonate ligands and phosphinoxides;
Exposure of the compounds to radiations on the Ultraviolet spectrum.

Resumo/Abstract

The optical properties of trivalent lanthanide ion (Ln^{3+}) coordination compounds are enhanced when the ions are coordinated with organic luminescence-sensitizing ligands. In this context, β-diketonate ligands are widely explored for the design of such. Due to their diverse technological applications, such as lasers, scintillators, and luminescent markers, some new technologies often require the exposure of the materials to high-energy beams. However, such radiation can cause the degradation of these complexes, especially in solutions. This occurs since sensitizing ligands exhibit a high potential for energy absorption in the ultraviolet (UV) region. Therefore, photo-redox processes, ionization of the central atom, or bond breakage of the complex can lead to reduced or complete suppression of its luminescence. Given this, this study reports the synthesis, characterization, and investigation of Eu^{3+} complexes photostability under different types of radiation, with the general formula $[Eu(\beta\text{-dic})_3(L)_2]$, where L corresponds to the auxiliary ligands (tpaso) and (tppo), and β-dic to the sensitizing ligands (btfa) and (tta). These complexes were characterized by CHN elemental analysis and Fourier transform infrared spectroscopy (FTIR). The results of the CHN show good agreement between the experimental and calculated values for the synthesized complexes. Furthermore, the FTIR data confirms the coordination of the metal atom to the sensitizing ligands. The emission spectrum is characterized by narrow bands associated with the intraconfigurational-4f6 transitions of the Eu^{3+} ion: $^5D_0 \rightarrow {}^7FJ$ (J: 0-4), being the band due to the $^5D_0 \rightarrow {}^7F_2$ transition the most intense one, resulting in the characteristic red-region emission. Currently, the samples are being submitted to UV and X-Ray emissions, in order to collect preliminary data about their photostability.

[1] Israel F. Costa, et. al., Coord. Chem. Rev., 502, 2024.

[2] Tatyana Emelina, et. al., Journal of Luminescence, 238, 2021.



Luminescence spectra of synthesized crystalline and solution complexes

Agradecimentos/Acknowledgments

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Influence of cellulose nanofibers on caffeine release profiles in calcium polyphosphate coacervates

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Palavras Chave:*Calcium polyphosphate coacervates, Cellulose nanofibers, Drug delivery, Caffeine.*

Highlights

Calcium polyphosphate coacervate as matrix for drug delivery; Biocompatible and synthesized at room temperature; Cellulose nanofibers improve structural stability and encapsulation efficiency.

Resumo/Abstract

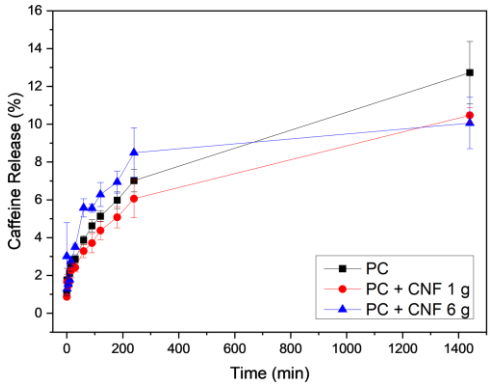
Polyphosphate coacervates (PCs) are highly versatile and biocompatible systems that can be prepared through a simple coacervation process by directly adding metal ion salt solutions to a concentrated $(NaPO_3)_n$ solution, without requiring organic solvents[1]. The PCs are prepared at room temperature, enabling the synthesis of inorganic-organic hybrid materials. Calcium polyphosphate coacervates (CaPCs) are highly hygroscopic, which may compromise their physicochemical stability and promote rapid drug release. The incorporation of biomolecules, such as cellulose nanofibers (CNFs), has been investigated as an effective strategy to enhance the stability of hybrid systems and modulate drug release behavior[2].

The CaPCs were prepared by simple coacervation, followed by addition of CNFs (1 g and 6 g). Caffeine (50 mg) was used as a model hydrophilic drug to evaluate the release performance of the CaPCs. In vitro release experiments were carried out using a dissolution apparatus at 37°C and 50 rpm in buffer solution (pH 7,4). Analysis showed incorporation efficiencies of 18,35%, 22,93%, and 22,56% for CaPC, CaPC+1 g CNFs, and CaPC+6g CNFs, respectively. The system without CNFs exhibited a faster cumulative caffeine release (12,73 ± 1,65), consistent with its higher hygroscopicity and lower structural stability. The incorporation of CNFs reduced the amount of caffeine released, with values of 10,47 ± 0,40 and 10,06 ± 1,36 for CaPC containing 1 g and 6 g of CNFs, respectively. Although the CaPC system with 6 g of CNFs showed a more pronounced initial burst release, it exhibited a more sustained release profile at longer times. These results indicate that the addition of CNFs influences both the initial and long-term release behavior of caffeine, contributing to improved control over drug release from polyphosphate coacervates.

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2. Breijaert, T.C.*et al.*Carbohydr. Polym. Technol. Appl., 10, 100756 (2025)



Caffeine release profiles comparing pure PC to PC containing different amounts of CNF (1 g and 6 g).

Agradecimentos/Acknowledgments

To the LAMF and LAVie research groups (IQAr-Unesp), BioPolMat group (UNIARA) and FAPESP (processes 2025/00095-9 and 2025/21216-9).

Influence of Synthesis Conditions on the Formation of NaYF4 Nanocrystals Via a Microwave-Assisted Method

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Palavras Chave:*Nanoparticles,Lanthanides,Rare Earths,Microwave*

Highlights

In this work, we demonstrate the influence of temperature, synthesis duration and solvents used in the structural properties of NaYF4 nanoparticles.

Resumo/Abstract

The $NaYF_4$ matrix has been studied recently mainly as a host material for luminescent lanthanides ions. This material can be prepared in two crystal structures, a cubic (α) and a hexagonal one (β). The low phonon energy of this material is one of the key points on its use as a host for lanthanide ions [1]. Therefore, developing new methods of synthesis, that yield nanocrystals of controlled size, morphology and crystal phase is essential.

A synthesis method already reported in the literature is the solvothermal one [2], and water, ethanol and oleic acid are used as solvents. One setback of this route is the need of long synthesis, reaching 24h. In order to reduce the synthesis duration, in this work we report the synthesis of $NaYF_4$ nanomaterials in a microwave assisted solvothermal method.

To optimize the conditions, both the synthesis duration and the temperature were varied. Our results indicate that shorter syntheses favor the cubic phase, while longer syntheses favor the hexagonal phase, as shown in Figure 1. Furthermore, lower temperatures lead to the formation of the cubic phase, as higher temperatures start to favor the hexagonal one. It was possible to obtain the pure α phase in a synthesis at 150°C for 30 min, but the pure β phase has not been obtained. Additionally, it has been carried out a series of syntheses with only oleic acid as the solvent at different temperatures, in which it has been observed the formation of ultrasmall α phase nanomaterials.

Therefore, it has been shown that synthesis conditions have a great impact on the nanomaterials' crystal phase, size, and morphology. Besides that, nanomaterials with similar characteristics of those prepared by the conventional solvothermal method were obtained with the microwave assisted method, but with much shorter synthesis.

[1] Chem. Rev. 2022, 5519, 122, 6 DOI: 10.1021/acs.chemrev.1c00644

[2] Langmuir 2015, 31, 7084 DOI: 10.1021/acs.langmuir.5b01151

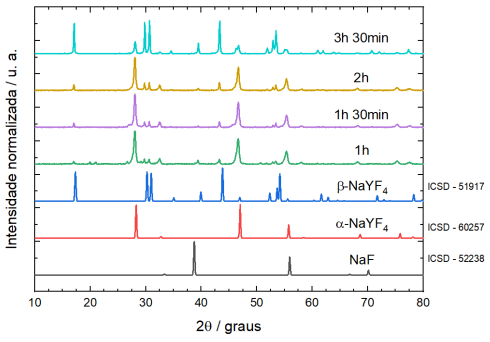


Figure 1 – XRD patterns of samples prepared at 200°C for different durations.

Agradecimentos/Acknowledgments

The authors are thankful for FAPESP (2021/08111-2 and 2025/01740-5), for CNPq and CAPES.

Investigação vibracional dos complexos catiônicos de Al(III) em acetonitrila e misturas binárias de solventes.

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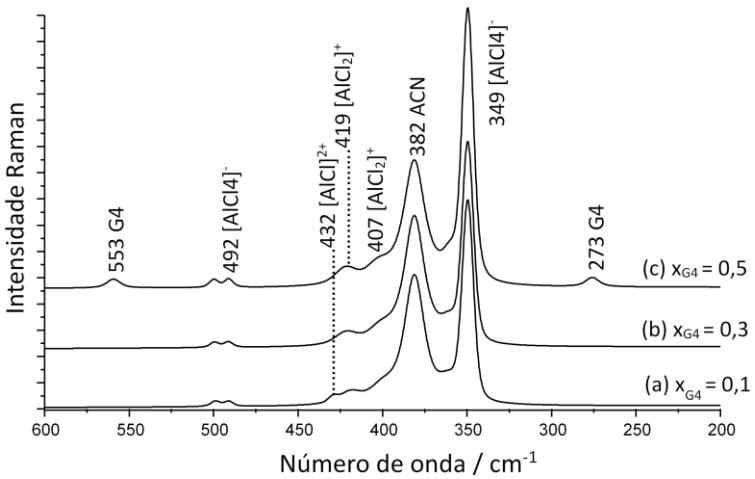
Palavras Chave:*Espectroscopia vibracional,cloreto de alumínio,acetonitrila,eletrólitos,especiação iônica.*

Highlights

Raman spectroscopy has identified for the first time the $[AlCl_2]^+$ cation in acetonitrile and in its binary mixtures containing tetraglyme.

Resumo/Abstract

Eletrólitos à base de nitrilas têm recebido atenção especial devido à notável estabilidade eletroquímica e térmica. A ligação C≡N, curta e polar, favorece a formação de íons e contribui para a condutividade do meio, tornando as nitrilas candidatas adequadas para baterias secundárias de alta densidade de energia. A acetonitrila (ACN) destaca-se por sua elevada estabilidade oxidativa e valor substancial de constante dielétrica (37,5), sendo capaz de dissociar efetivamente diferentes sais. De fato, estudos anteriores reportaram a formação de espécies iônicas em soluções de $AlCl_3$/ACN, muito embora ainda exista uma lacuna na identificação vibracional segura dos complexos catiônicos de Al(III). No presente trabalho, espectroscopia Raman foi usada para a especiação de $AlCl_3$em ACN e os efeitos da adição de tetraglima (G4). Na mistura rica em ACN (Figura 1(a)), uma banda em 432 cm^{-1}, já observada e atribuída por outros autores aos complexos $[AlCl(ACN)_5]^{2+}$ e $[Al(ACN)_6]^{3+}$, está presente no espectro, mas desaparece quando a fração molar de G4 (xG_4) aumenta (Figuras 1(b);(c)). Ao mesmo tempo, duas bandas em 419 e 407 cm^{-1} têm suas intensidades aumentadas e suas posições são muito próximas daquelas identificadas por nosso grupo no solvente G4 (420 e 400 cm^{-1}). Essas duas bandas são, portanto, atribuídas ao complexo $[AlCl_2(ACN)_x(G4)y]^+$ e confirmam a estabilização de espécies de carga positiva mais baixa em função do decréscimo da constante dielétrica do meio. Nosso resultado reforça que o cátion monovalente é o ácido de Lewis preferencialmente formado nos eletrólitos do tipo MACC ($MgCl_2/AlCl_3$), sendo, de fato, o responsável pela corrosão do ânodo de Mg em baterias recarregáveis.



Espectros Raman de AlCl3–ACN:G4 (2,0 molal), na região Al–ligante, para xG4 = 0,1; 0,3; 0,5.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG, UFJF

Investigation of a neutral triruthenium complex reactivity with molecular oxygen: a potential new agent for photothermal therapy

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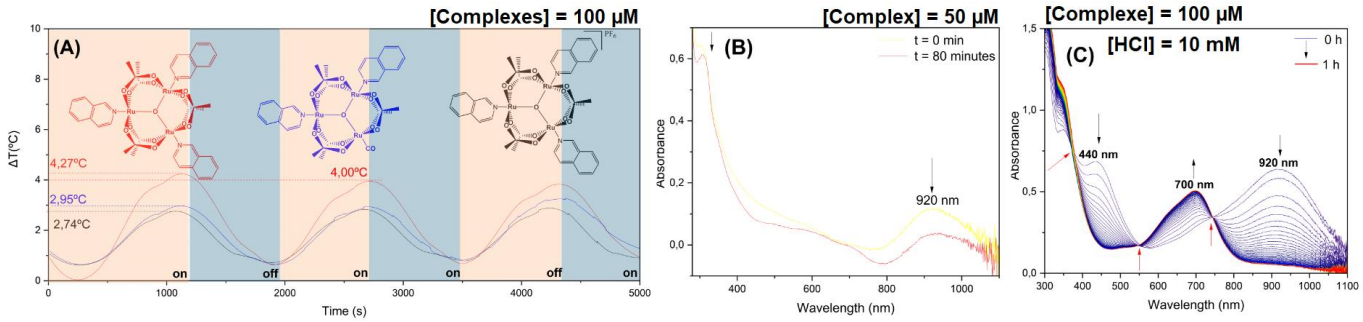
Palavras Chave:*Photothermal therapy; redox reactivity; oxygen; ruthenium complex; isoquinoline*

Highlights

The complex $[Ru_3O(CH_3COO)_6(L)_3]$ showed potential as a photothermal agent, but its instability in aerated solutions made an investigation of its redox reactivity necessary to evaluate viability.

Resumo/Abstract

A photothermal agent is a molecule, material, or structure that converts light radiation into heat.[1] These agents can be used in a wide range of applications, including photothermal therapy (PTT), where thermal ablation is generated through irradiation on photothermal agents in the near-infrared region (700-1100 nm).[1] On this base, complexes from the triruthenium cluster class were tested as photothermal agents. These are non-emissive compounds,[2] which could be an advantageous property, once there is no competition with other radiative decay processes. This premise was tested by measuring the temperature increase of water solutions (100 µM) of the complexes $[Ru_3O(CH_3COO)_6(isoquinoline)_3]PF_6$, $[Ru_3O(CH_3COO)_6(isoquinoline)_3]$ and $[Ru_3O(CH_3COO)_6(isoquinoline)_2CO]$ with 2% of dimethyl sulfoxide (%v/v) irradiated at 808 nm. The temperatures were measured with a fiber optic thermometer, and three consecutive cycles with (on) and without (off) irradiation were measured (figure 1A). The complex $[Ru_3O(CH_3COO)_6(isoquinoline)_3]$ showed a temperature increase within the range expected for PTT applications (4-8 ºC),[1] with 4,27 ºC after 13 minutes and 6,30 ºC after 20 minutes of irradiation. Despite the positive result, this compound, as others $[Ru_3O(CH_3COO)_6(L)_3]$, is not long-term stable in aerated solution.[2] Due to this limitation, its reactivity with molecular oxygen was studied. In 50 µM aerated aqueous solution (Figure 1B) compound oxidation ($[RuIII,III,II_3O(CH_3COO)_6(isoquinoline)_3]$ to $[RuIII,III,III_3O(CH_3COO)_6(isoquinoline)_3]^+$) was observed after 80 minutes, following electronic spectra changes. In acetonitrile 100 µM solution, oxidation was achieve after 65 h in a non-acidified medium and in 1 hour in acidified medium (figure 1 C) with 10 mM HCl, with kinetics constants of (2,98 ± 0,89) x 10^{-5} s^{-1} and (2,98 ± 0,89) x 10^{-5} s^{-1}. Further studies will be developed in order to understand this process.
References are along with acknowledgments.



Temperature rise of aqueous triruthenium complexes (A) and reactivity in water (B) and acid organic

Agradecimentos/Acknowledgments

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Investigation of the Interaction Between the Herbicide Imazaquin and Copper(II) Ions: Electrochemical, Spectroscopic, and Computational Studies

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Palavras Chave:*Complexos de Cobre(II),pesticida,Imazaquim,Química Computacional,Espectroscopia*

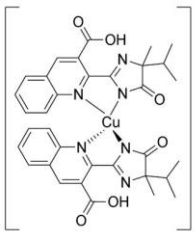
Highlights

Investigation of the complexation between environmental pollutants in aqueous medium: Cu^{2+} and imazaquin. Determination of the [1:2] stoichiometry by electrochemical and computational techniques.

Resumo/Abstract

Imazaquin (IMZ), an imidazolinone herbicide widely employed for weed control in Brazilian soybean crops, possesses a carboxylic moiety susceptible to dissociation in edaphic environments, generating anionic species capable of interacting with metal ions. Copper, a metal of significant environmental interest, exhibits high affinity for ligands containing oxygen and nitrogen, which favors the concomitant formation of complexes with pesticides bearing such functional groups. This work investigated the interaction between IMZ and the copper(II) ion (Cu^{2+}) using electrochemical techniques, spectroscopy, and quantum chemical calculations. Experiments were conducted in 0.1 mol L^{-1} Britton-Robinson buffer (pH 2.0), employing a pencil lead graphite electrode as the working electrode. Cyclic voltammetry revealed a shift in potentials toward more negative values, indicative of copper complex formation. Experimental data suggest a [1:2] stoichiometry for the $[Cu(IMZ^{-})_2]$ complex. This ratio was corroborated by quantum calculations, performed in Gaussian 09 utilizing B3LYP/6-311G(d,p), which allowed for the proposition of a molecular structure with a binding energy (ΔE) of –2616.44 kJ·mol^{-1}, demonstrating high thermodynamic stability and classifying it as the most stable complex among the theoretical models evaluated (Table 1). The calculations also enabled the prediction of infrared (IR) spectroscopic parameters, subsequently confirmed experimentally following complex synthesis. The spectra displayed bands consistent with the predicted vibrational modes, associated with N–H (3400–3200 cm^{-1}), C=O (1720–1700 cm^{-1}), and C–N (1600–1580 cm^{-1}) stretching. The disappearance of the band at 1000 cm^{-1} (assigned to the imidazolinone ring vibrational mode) was observed, corroborating the involvement of nitrogen atoms in the coordination sphere of the Cu(II) metallic center and confirming the formation of N–N chelates, suggesting the structure presented in Figure 1.

Complexo 3 – $[Cu(IMZ^{-})_2]$



Complex	Coordination Formula	Ligand state	Deprot.	Energy (kJ/mol)
1	$[Cu(IMZ)(H_2O)2]^{2+}$	IMZ neutral + H_2O	No	-1333,97 kJ/mol
2	$[Cu(IMZ)_2]^{2+}$	IMZ neutral	No	-1325,60 kJ/mol
3	$[Cu(IMZ^{-})_2]$	IMZ desprot. (N-N)	Yes (N-H)	-2616,44 kJ/mol

Proposed molecular structure for the [Cu(IMZ-)2] complex

Agradecimentos/Acknowledgments

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Investigation of the reuse capacity of the layered solid cobalt hydroxide chloride salt as catalyst to Brilliant Green degradation

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Palavras Chave:*Layered hydroxide salts,Organic dyes,Green chemistry,Heterogeneous catalysis*

Highlights

Synthesis and characterization of the layered cobalt hydroxide chloride salt. Promising catalytic results in terms of catalyst reusability in the bleaching reaction of Brilliant Green organic dye.

Resumo/Abstract

The solid layered cobalt hydroxide chloride material (HClCo), belonging to the family of the layered hydroxide salts [1], was prepared, structurally characterized, and evaluated as catalyst to the oxidative bleaching of the environmentally relevant dye Brilliant Green (BG) [2], employing hydrogen peroxide as the oxidizing agent. The HClCo phase was prepared by a modified ammonia diffusion approach [3], carried out in a sealed desiccator containing aqueous cobalt(II) nitrate solution (0.1 mol L^{-1}) and concentrated ammonia solution (10.4 mol L^{-1}) for seven days. The resulted solid was characterized by powder X-ray diffraction (basal spacing of 7.99 Å), infrared spectroscopy (bands below 1000 cm^{-1} attributed to Co–O lattice vibrations and a broad absorption centered at 3498 cm^{-1} assigned to O–H stretching of interlayer water molecules), scanning electron microscopy, and X-ray photoelectron spectroscopy (XPS). The XPS results confirmed the exclusive presence of Co^{2+} species, consistent with the material's classification as a layered hydroxide salt. The combined analyses verified the successful formation of the HClCo phase. The catalytic performance of HClCo was investigated in the degradation of BG in aqueous. Compared to control experiments results just BG + hydrogen peroxide) conducted under identical preliminary conditions (25 °C, magnetic stirring, with and without ambient light), the presence of the catalyst solid significantly enhanced the dye bleaching rate. Nearly complete discoloration (~100%) was achieved using HClCo solid as catalyst. Recycling experiments at same conditions demonstrated that the catalyst preserved its high activity, maintaining degradation efficiencies above 98% up to the fifth reuse cycle. Studies are currently being conducted to identify the degradation products and to elucidate the possible reaction pathways involved in the oxidative process.

Agradecimentos/Acknowledgments

CAPES, CNPq, Fundação Araucária e Instituto Nacional de Ciência e Tecnologia em Ciências Moleculares (INCT-CiMol) e à Profa. Dra. Maria Luiza Rocco (UFRJ) pela realização das análises de XPS.

Isostructural Calixarene-Like Lanthanide Magnets Based on Gd(III), Dy(III) and Tb(III) Oxamate Complexes

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Palavras Chave:*supramolecular chemistry,gadolinium(III),terbium(III),dysprosium(III),molecular magnetism.*

Highlights

Three new mononuclear Gd(III), Dy(III), and Tb(III) phenyl(oxamato) complexes, as well as their precursor salt, are synthesized and characterized.

Resumo/Abstract

Complexes of lanthanide(III) ions are an attractive source of multifunctional materials since they can combine luminescent functionalities with magnetic properties[1]. This work presents the synthesis and chemical/structural characterization of three new air-stable isostructural compounds of formula***n*-Bu$_4$N[Ln(Hphox)$_4$(DMSO)]·2H$_2$O**[Hphox = phenyloxamate; DMSO = dimethyl sulfoxide; Ln = Gd^{3+}(**1**), Dy^{3+}(**2**) and Tb^{3+}(**3**)]. These complexes were obtained through the reaction of the salt, tetrabutylammonium phenyl(oxamate) (*n*-Bu_4NHphox), and the trivalent rare earth metal ions in a 4:1 ligand-metal molar ratio. The salt was characterized by elemental analysis and IR spectroscopy, and its molecular formula was confirmed by ^{1}H and ^{13}C NMR spectroscopy. Complexes**1**-**3**were characterized by elemental analysis, thermogravimetric analysis, infrared spectroscopy, and X-ray diffraction patterns (PXRD). Single-crystal X-ray diffraction analysis reveals the crystalline structure of**2**. It consists of calixarene-type monoanionic species containing all-*cis*-disposed Hphox ligands and one DMSO molecule coordinated to the Dy^{3+} ion, featuring a nine-coordinated environment, in addition to two water molecules of crystallization. The tetrabutylammonium cations are situated between the anionic units, and the aromatic rings of mononuclear structures upwards and downwards. The smallest distance between the Dy•••Dy ions in**2**is 10.971 Å (Figure 1), closer than reported for other oxamate compounds previously reported.[2]The comparison between the PXRD simulated from the crystal structure of**2**and the experimental ones of**1**and**3**suggests that all compounds are isostructural. Preliminary results show that**3**exhibit visible luminescence at room temperature under UV irradiation. Studies of the magnetic and photoluminescent properties of**1**-**3**will be carried out.

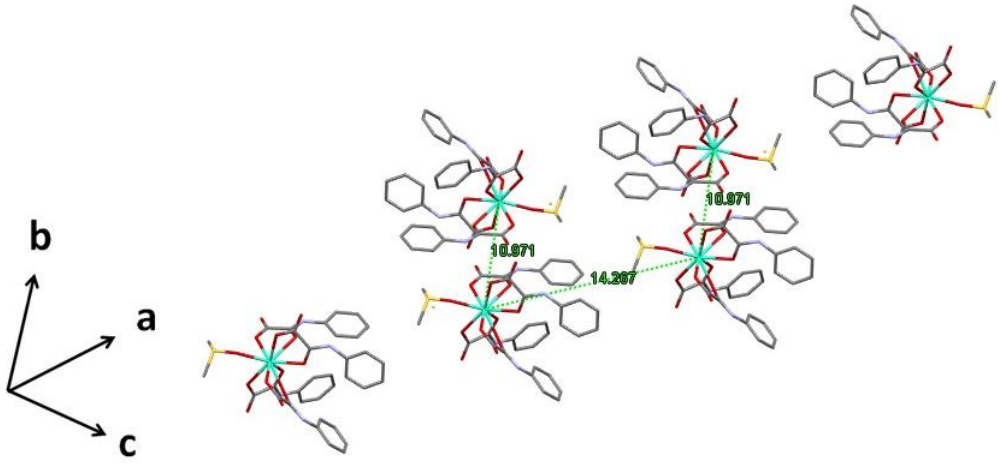


Figure 1 Representation of anionic crystalline structure of 2

Agradecimentos/Acknowledgments

CNPq; FAPEMIG; CAPES; LabCri/UFMG; Synthares/UFMG; NEPS DQ/UFMG; CEFET-MG.

Kinetic Effects on Size and Stability of Citrate-Stabilized Rare-Earth Vanadate Nanoparticles.

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Palavras Chave:*Rare-Earth Vanadate Nanoparticles,Size,Citrate,Stability,Kinetic Effects*

Highlights

Citrate-stabilized YVO_4:Eu NPs lose colloidal stability at low pH. Over time, NPs show zeta potential decay and slight aggregation.

Resumo/Abstract

Rare-earth vanadate nanoparticles (NPs) exhibit luminescence under ultraviolet and near-infrared excitation, as well as tunable morphology, composition, and surface functionalization, enabling applications in sensing, nanothermometry, bioimaging, and catalysis.[1] These properties can be enhanced and combined through the controlled assembly of NPs into more complex structures (supraparticles), enabling multiple properties within a single system. In this context, YVO_4:Eu NPs (~10 nm) were synthesized using citrate as a surface stabilizing agent,[2] to investigate their colloidal stability under pH variation (2–12) and temporal aging of the suspensions, to define methods for later aggregation.

At pH≤4, protonation of the citrate carboxylate groups occurs, reducing electrostatic stabilization and leading to aggregation. At pH=2, aggregation into micrometric structures takes place, possibly accompanied by partial dissolution of the NPs, as reported for similar systems in literature.[3], [4]

At pH=7, the NPs remained stable for 14 days after synthesis, however, zeta potential became less negative, from ζ~−57 to ζ~−30 mV, indicating reduced electrostatic stabilization over time. Despite this, the hydrodynamic diameters remained nearly constant, with an increase from 9±2nm to 13±3nm, due to the Ostwald ripening process.

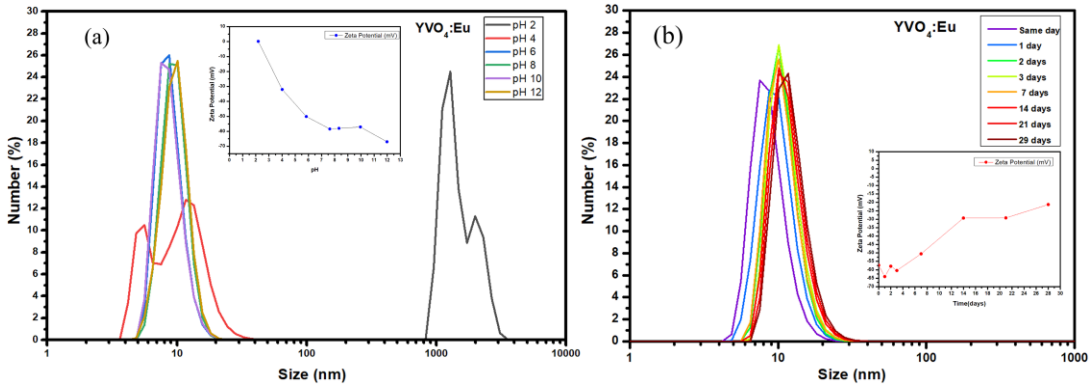
It can be concluded that lowering the pH allows partial aggregation of the NPs, although there is competition with solid dissolution, which directly affects their compositional stability, whereas at pH=7 aging leads to reduced surface charge without significant aggregation. Understanding pH-dependent colloidal behavior provides a basis for developing ligand-exchange strategies and controlling NPs surface interactions and structural organization.

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3.Yazdani, S. et al. ACS Omega 2021, 6, 16847-16853.

4.Sati, A. et al. ACS Omega 2025, 10, 7549-7582.



a) Size distribution vs pH (2–12); b) size distribution vs time and respective zeta potentials.

Agradecimentos/Acknowledgments

CAPES, FAPESP (2022/03442-3), CNPq (proc. nº 144777/2025-8) and LISpec (RRID:SCR_027391).

Kinetics of Nucleophilic Addition of Sulfite ions to Ruthenium Nitrosyl Complexes

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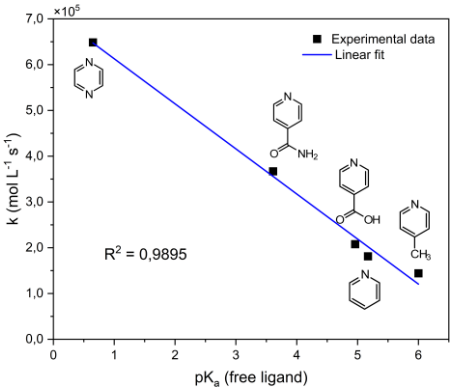
Palavras Chave:*Ruthenium(II) nitrosyl complexes,Nucleophilic addition,Chemical kinetics,Stopped-flow spectroscopy,Ligand effects*

Highlights

Kinetic study of sulfite addition to RuII–NO^+ complexes. Fast reactions monitored by stopped-flow UV–Vis spectroscopy. Linear correlation between rate constants and ligand pK_a values.

Resumo/Abstract

This work investigates the kinetics of nucleophilic addition reactions in hexacoordinate ruthenium(II) nitrosyl complexes of the general formula*trans*-[RuII$(NH_3)_4$(L)(NO^+)]$^{3+}$, bearing different ligands trans to the nitrosyl group to correlate {$RuNOSO_3$} formation rate constants with ligand properties. The nucleophilic addition of sulfite (SO_3^{2-}) was studied for complexes with L = pyrazine, pyridine, 4-picoline, isonicotinic acid, and isonicotinamide, yielding the corresponding nitrosylsulphito adducts*trans*-[RuII$(NH_3)_4$(L)$(N(O)SO_3)$]$^+$. The reactions were monitored by stopped-flow UV–Vis spectroscopy. Kinetic studies were conducted under pseudo-first-order conditions, using an excess of sulfite relative to the complex (C = 50 µM), in pH 7.4 at ionic strength 0.22 M. The kinetics results obtained for trans-[RuII$(NH_3)_4$(L)(NO^+)]$^{3+}$ were dependent on the nature of the ligand trans to NO, with rate constants following the order of 10^5 M^{-1} s^{-1}. Previous literature reports indicate that the reactivity of this class of complexes can be correlated with electronic parameters such as NO^+/NO^- redox potentials and Lever electrochemical parameters. In the present study, attempts to correlate the experimental rate constants with these parameters did not yield satisfactory linear relationships, resulting in coefficients of determination (R^2) in the range of 0,59 – 0,75. In contrast, a strong linear correlation was observed between the rate constant k and the pK_a of the conjugated acids of the ligands (L), with a R^2 ~0,99. These results indicate that less basic ligands enhance the electrophilic activation of the {RuNO} fragment, thereby facilitating nucleophilic attack and formation of the final nitrosylsulphito adduct. Overall, these findings highlight the relevance of structure-reactivity relationships and demonstrate that ligand basicity is a key parameter for understanding and predicting the reactivity of ruthenium(II) nitrosyl complexes based on their molecular structures.



Plot of k versus pKa of the free ligand for trans-[RuII(NH3)4(L)(NO)] complexes.

Agradecimentos/Acknowledgments

The authors acknowledge FAPESP (processes 2025/13566-0 and 2025/09383-7) , as well as CNPq and CAPES for their financial support.

Lanthanide-Based Luminescent Markers: A Novel Approach to Public Safety and Forensic Autopsy

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Palavras Chave:*Luminescent markers,Lanthanide luminescence,Forensic autopsy,Public Safety,Lanthanide Metal–organic frameworks (LnOFs)*

Highlights

Lanthanide coordination compounds were synthesized as luminescent markers for firearm ammunition.

Ballistics tests confirmed their use in crime elucidation and necropsy procedures.

Resumo/Abstract

Mixed coordination compounds of lanthanides can be synthesized with different molar fractions of two or more metal ions. Due to their spectroscopic properties, these materials have been widely investigated as markers in firearm ammunition. This work reports the synthesis, structural, and photophysical characterization, and application of four new mixed lanthanide-organic frameworks (m-LnOFs) and one mixed discrete lanthanide complex as luminescent markers for ammunition used in pistols and rifles. The m-LnMOFs were synthesized by a hydrothermal method using 1,2,4,5-benzenetetracarboxylic acid (Hbtec) and different molar fractions of Eu^{3+}, Tb^{3+}, and Gd^{3+}, yielding $[Eu_{0.007}Gd_{0.3}Tb_{0.693}(Hbtec)]_n$**(1)**, $[Eu_{0.014}Gd_{0.8}Tb_{0.186}(Hbtec)]_n$**(2)**, $[Eu_{0.014}Gd_{0.9}Tb_{0.086}(Hbtec)]_n$**(3)**, and $[Eu_{0.0167}Tb_{0.9833}(Hbtec)]_n$**(4)**, applied to different rifle and pistol calibers. The discrete complex $[Eu_{1.8}Tb_{0.2}(ceto)_6(bpy)_2]$**(5)**was incorporated into hollow-point ammunition. Upon impact, the projectile deforms, gradually releasing the marker, which can be identified using a simple ultraviolet light lamp. This enables the estimation of the ballistic trajectory, the precise location of the projectile, and, consequently, the cause of death, while also expediting necropsy analyses. Ballistics tests confirmed effective marker incorporation and distinct spectroscopic fingerprints. All compounds were characterized using different analytical and spectroscopic techniques. Photoluminescence studies showed efficient ligand-to-metal energy transfer, producing tunable green, yellow, orange, and red emissions depending on the Eu^{3+}/Tb^{3+} ratio. Thus, the compounds presented herein proved to be efficient luminescent markers for firearm ammunition, with potential applications in crime elucidation and in expediting forensic autopsy analyses.



Hollow-point projectile applied to autopsy analysis and m-LnOFs as selective firearm markers

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Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq)

Luminescent films combining a EuIII complex and a persistent luminescent phosphor displaying dual color encoding for anti-counterfeiting applications

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Palavras Chave:*Lanthanides,Rare earths,Luminescence,Anti-Counterfeiting,Coordination chemistry*

Highlights

PMMA films containing a EuIII β-diketonate complex and persistent luminescent phosphor;

Dual temporal and spectral encoding depending on the excitation wavelength and time.

Resumo/Abstract

Luminescent anti-counterfeiting systems operate based on modulated emission upon external stimuli, such as light or heat, playing a fundamental role in the protection of banknotes, artworks, and other products. However, as the known systems become easier to replicate, the development of more complex reproduction methods that require greater technical expertise becomes increasingly important. Herein, it is presented the development of multicolor luminescent polymeric films based on poly(methyl methacrylate) (PMMA) featuring spectral and temporal coding for advanced anti-counterfeiting applications. The films combine the $SrAl_2O_4$:EuII,DyIII phosphor, which exhibits persistent luminescence in the green spectral region, and the red-light-emitting complex [Eu(nta)$_3$(phen)] (nta: 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione; phen: 1,10-phenanthroline). The films display several features: optical transparency, homogeneous dispersion of the luminescent activators, and excitation within the near-UV spectral window. In these films, the emission color shifts from red to green as the excitation wavelength varies from 380 to 440 nm, due to the favoring of the $SrAl_2O_4$:EuII,DyIII persistent luminescence. Furthermore, under 380 nm excitation, the red emission, dominated by the EuIII complex, transitions to green after the excitation source is switched off, owing to the persistent luminescence of $SrAl_2O_4$:EuII,DyIII. Upon UV excitation, the films exhibit an emission quantum yield close to 60% and remain thermally stable up to 200 °C. Our results show that the combination of conventional and persistent luminescent materials in a polymeric matrix allows for dual-mode luminescence encoding with spectral and temporal resolution. This is a simple approach, but difficult to be reproduced without specialized knowledge, favoring its application in anti-counterfeiting.[1]

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Agradecimentos/Acknowledgments

To FAPESP for the scholarship provided to TPP (2025/04765-9). AGBJ thanks the Support Program for New Faculty at USP from PRPI - USP.

Luminescent Lanthanide Tetrakis Complexes as Promising Dopants for Luminescent Solar Concentrators

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Palavras Chave:*Tetrakis,lanthanides,Luminescent Solar Concentrators*

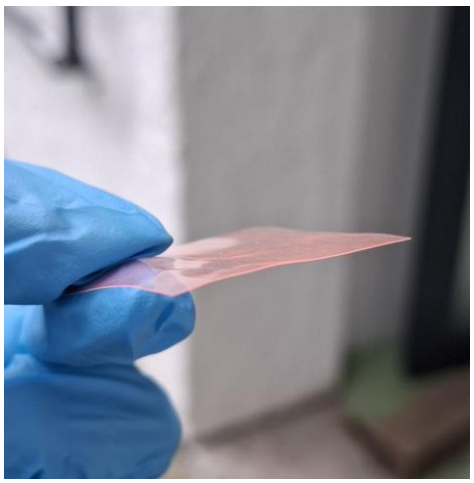
Highlights

Promising materials for luminescent solar concentrators and solar energy conversion.

Europium complex shows strong antenna effect and intense UV-driven luminescence.

Resumo/Abstract

complexes based on β-diketone ligands are well documented due to their ability to sensitize Ln^{3+} ions through the antenna effect, leading to luminescent materials with high quantum yields. These materials show potential applications in several technological areas, including optical markers and biocompatible probes for imaging. Considering the growing demand for green energy and high-performance alternatives for electricity generation, luminescent solar concentrators (LSCs) have attracted academic interest for decades because of their ability to enhance the conversion efficiency of photovoltaic cells. Lanthanide-based materials are promising for LSCs, as they efficiently interact with solar radiation (UVA, UVB, and UVC) when used as dopants in polymer films. In this work, tetrakis complexes containing the unusual counterion methyltriphenylphosphonium (MTPP) and the ligand thenoyltrifluoroacetonate (tta) were synthesized via a one-pot method. The resulting compounds, with the general formula $MTPP[Ln(tta)_4]$ (Ln = Eu^{3+}, Tb^{3+}, Gd^{3+}), were characterized by single-crystal X-ray diffraction, elemental analysis, and thermal analysis. Photophysical investigation based on excitation and emission spectra revealed an efficient antenna effect for the europium complex. As a preliminary test, a PMMA film doped with 1% (w/w) Eu^{3+} was prepared, demonstrating the potential of these complexes for LSC applications, as the film exhibits visible emission under sunlight even in cloudy weather.



PMMA film doped with 1% of Europium complex exposed in cloudy weather

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Magneto-Luminescent Hybrid Nanomaterials with Dual-Mode Optical Emission for Advanced Anti-Counterfeiting Inks

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Palavras Chave:*Multifunctional Nanomaterials, Security Devices, Magnetic Nanoparticles, Nanobiotechnology, Multimodal Excitation.*

Highlights

A magneto-luminescent $Fe_3O_4/Y_{1.76}Yb_{0.20}Er_{0.04}O_3@SiO_2$-[Eu(dbm)$_3$(pamba)] hybrid ink was developed, combining magnetic response with excitation-dependent luminescence.

Resumo/Abstract

Recent progress in multifunctional hybrid has enabled the design of advanced anti-counterfeiting systems based on the integration of complementary authentication mechanisms. In this study, a magneto-luminescent hybrid with the $Fe_3O_4/Y_{1.76}Yb_{0.20}Er_{0.04}O_3@SiO_2$-[Eu(dbm)$_3$(pamba)] architecture for application in functional security inks was synthesized and optimized following a previously reported methodology[1]. Structural and morphological analyses confirmed the successful deposition of the silica shell. Microscopic observations revealed a core@shell architecture surrounded by a silica layer, while magnetic measurements indicated that the ferrimagnetic nature of the Fe_3O_4 core is preserved after coating, although with reduced saturation magnetization. Optical investigations revealed dual emission behavior governed by the excitation wavelength. Near-infrared excitation at 980 nm produces orange upconversion emission associated with Er^{3+}, with a color purity to 99.1%, whereas ultraviolet excitation at 340 nm yields red downshifting emission arising from efficient ligand-to-metal energy transfer to Eu^{3+},with a color purity of 99.6%[2]. Notably, both luminescent responses persist after incorporation of the hybrid material into a poly(vinyl alcohol) matrix, forming a processable ink. The resulting ink also preserves magnetic activity, enabling simultaneous magnetic and optical readout. So, this study establishes a hybrid ink platform that integrates magnetic and luminescent functionalities within a single formulation, overcoming limitations of conventional lanthanide-based anti-counterfeiting systems. The proposed strategy provides a coherent and versatile framework for advanced anti-counterfeiting technologies based on multimodal verification.

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[2]ZHENG, B.*et al*. Chemical Reviews, v. 122, n. 6, p. 5519-5603, 2022.

Agradecimentos/Acknowledgments

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Mechanoluminescent and Photoluminescent Properties of Tb^{3+} Complexes Containing a Phenylacetate Ligand

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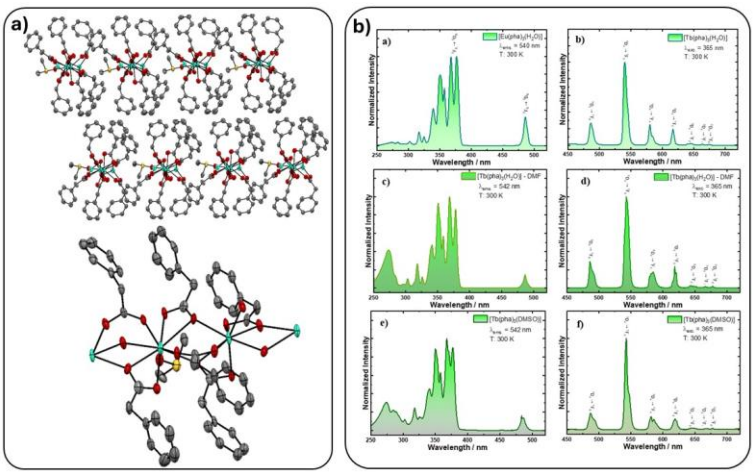
Palavras Chave:*Luminescence,mechanoluminescence,terbium,phenylacetate,lanthanides*

Highlights

Polymeric Tb^3–phenylacetate complexes synthesized using H_2O, DMSO, and DMF as solvents. Study of mechanoluminescent and photoluminescent properties

Resumo/Abstract

Mechanoluminescence (ML) is the phenomenon of light emission induced by the application of mechanical stimuli to solid materials. Actions such as compression, stretching, cleavage, and grinding can trigger this effect, as they promote excitation processes that result in light emission. [1] In this context, this work explores the influence of the solvent on the photoluminescence (PL) and mechanoluminescence (ML) properties of complexes containing the phenylacetate (pha) ligand, with the general formula $[Tb(pha)_3(L)]$, where L : H_2O, DMF, and DMSO. The compound $[Tb(pha)_3(H_2O)]\infty$ was synthesized via direct reaction between the sodium salt of phenylacetic acid and a terbium salt in dilute aqueous solution, and part of the material was recrystallized in DMSO and DMF by slow evaporation.[2] The complexes were characterized by FT-IR spectroscopy and CHN microanalysis, and the results indicated the formation of the complexes with the proposed formula. The structure of the DMSO containing complex was elucidated by single crystal X-ray diffraction; this compound crystallizes in the monoclinic crystal system, space group Pc (Fig 1a). It is worth noting that the H_2O-containing complex is not isostructural with the others; this was confirmed by powder X-ray diffraction, which shows different diffraction patterns. Subsequently, the excitation spectra of the compounds were recorded and evaluated based on the intensity relationship between the ligand bands and the 4f–4f transitions. The emission spectra showed the absence of the ligand's broad emission band and the presence of the characteristic sharp bands of the $^5D_4 \rightarrow {}^7FJ$ transitions (J = 0–6), confirming the efficient sensitization of the Tb^{3+} ion (Fig 1b). The ML emission spectrum could not be recorded directly; however, the phenomenon was documented by video and by emission spectroscopy for the DMSO-containing complex.



a) Structure of the $[Tb(pha)_3(dmso)]\infty$ complex. b) Excitation and emission spectra of the complex.

Agradecimentos/Acknowledgments

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Metal-Saccharin Complexes Applied as Antimicrobial Inorganic Pigments for Surface Protection

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Palavras Chave:*Iron,Cobalt,Nickel,Copper,Antimicrobial*

Highlights

Inorganic synthesis of metal-saccharin complexes; Application as pigments in furniture paints; Antimicrobial and antifungal testing.

Resumo/Abstract

The pandemic and post-pandemic period (2020-2023) spurred investigations into new compounds with antifungal, antimicrobial, and antiviral activities. New compounds can result from interactions between transition metals and ligands, thereby forming metal-ligand complexes. In 2023, we began adapting the synthesis protocol using the saccharin ligand.

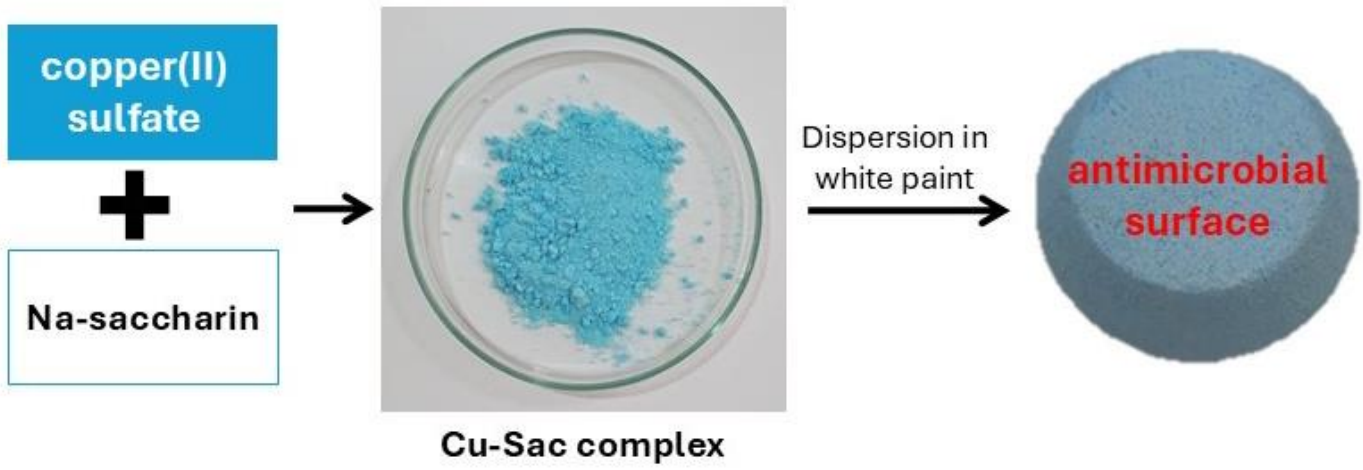
The compound 1,2-benzothiazole-3(2H)-one, 1,1-dioxide, commercially known as saccharin, discovered in 1878, is widely used as an artificial sweetener and food additive. We therefore assume that it is a non-toxic binder for the human body and can be ingested in daily quantities established by the manufacturer.

The synthesis of metal-saccharin complexes is straightforward and widely used in undergraduate coordination chemistry courses as an experimental procedure. Starting with aqueous solutions of the ligand and the inorganic salt of the metal of interest (Fe, Co, Ni, Cu), they are combined in a metal-ligand ratio (1:2), resulting in the M-Sac complex.

The solid M-Sac was characterized by mass spectrometry (MS), vibrational (FTIR) and electronic (Vis) spectroscopy, single-crystal X-ray diffraction (SCXD), thermal analysis (TG/DTA), and colorimetry (CIE L*a*b*).

The evaluation of antimicrobial potential was performed in different forms (tablets, solution, and dispersed in ink) using the diffusion disk and microdilution tests. The evaluation begins with the minimum inhibitory concentration (MIC) assay, selecting strains of Gram-positive and Gram-negative bacteria; and pathogenic or phytopathogenic fungi. The methodology defined by the Clinical and Laboratory Standards Institute was followed.

The results and discussions were published in the articles Cu-Sac (http://dx.doi.org/10.1016/j.jinorgbio.2025.112990) and M-Sac (http://dx.doi.org/10.1021/acsomega.5c07778).



Scheme of the formation of the blue Cu-Sac complex, dispersed in ink for application as a pigment.

Agradecimentos/Acknowledgments

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Modulation of biological potential of 4-aminobenzoic hydrazide by its coordination

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Palavras Chave:*Cytotoxic profile; hydrazide; structure-activity*

Highlights

Structural modification impact directly on cytotoxicity of hydrazide-based species.

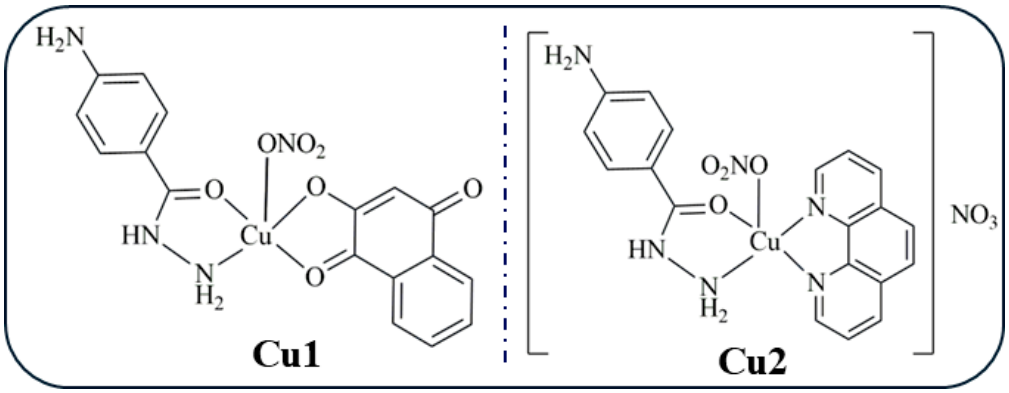
Copper compounds with hydrazides have been showing significant*in vitro*biological profile.

Resumo/Abstract

Hydrazides and their derivatives have recognized biological activity in the literature. For example, 4-nitrobenzohydrazide and benzohydrazide have great activity against chronic myelogenous leukemia cell line (K562).[1] Hydrazides structural modifications can improve the activity, whether by organic derivatives or coordination to metal center.[2] This result is evidenced in the present work. We compare the cytotoxic activity from 4-aminobenzoic hydrazide (**4-AMNH**) with two novel copper complexes containing 4-AMNH and lawsone or 1,10-phenanthroline, designated by**Cu1**and**Cu2**, respectively. The complexes were characterized by elemental analysis, infrared and UV-vis spectroscopy, which corroborate the proposed structures. The cytotoxicity evaluation was conducted against some squamous carcinoma and melanoma cell lines (hypopharyngeal squamous cell carcinoma – FaDu; tongue squamous cell carcinoma – SCC25; human melanoma cell lines – A375 and SK-MEL-28). A non-tumoral cell line was employed, immortalized human keratinocyte (HaCaT). It was possible to determine that**4-AMNH**did not present activity at the concentrations used (IC_{50} > 200 µM), whereas**Cu2**showed a marked activity against the SCC25 and SK-MEL-28 cell lines (IC_{50} ~ 5 µM). In contrast,**Cu1**showed activity only against the FaDu cell line (IC_{50} > 20 µM). These findings suggest that modifications resulted in different mechanisms for the compounds. To investigate this possibility, some experiments to evaluate potential interaction with some biomolecules are being carried out. In summary, the hydrazide-based complexes show potential for further investigations, as studies on their mechanisms of cell death and evaluation in animal models. Organic derivatives of 4-AMNH have been synthesized to generate new complexes and thereby broaden the structure-activity relationship.

[1]Oliveira, L.P.,*et al*.**Journal of Molecular Structure**, 2019;

[2]Teixeira, S.,*et al.***Molecules**, 2025.



Proposed structure for complexes Cu1 and Cu2

Agradecimentos/Acknowledgments

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Modulation of Vibrational and Luminescence Signals by Gold Nanoparticles in the Raman Spectrum of PMMA Films containing a EuIII complex

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Palavras Chave:*Lanthanides,Rare earths,Coordination chemistry,Materials chemistry*

Highlights

Plasmonic effect played by Au nanoparticles influences the intensity of Raman and luminescence bands monitored through Raman spectroscopy

Resumo/Abstract

Raman spectroscopy is a powerful tool to monitor temperature at the nanoscale. Our group showed that temperature can be monitored by a ratiometric thermometric parameter based on the ratio of vibrational-to-luminescence bands commonly detected by Raman spectroscopy. For that, a EuIII β-diketonate complex was dispersed in poly(methyl methacrylate) (PMMA), and the intensity ratio between a PMMA vibrational band and the EuIII luminescence was monitored.[1] To further investigate how this feature can be tuned, the [$Eu(btfa)_3(phen)$] complex (phen: 1,10-Phenanthroline; btfa: 4,4,4-trifluoro-1-phenyl-1,3-butanedionate) was dispersed in PMMA, and Au nanoparticles (NPs, size of 20 nm, plasmon at 522 nm) were incorporated to evaluate how the vibrational-to-luminescence signal is affected by the plasmonic effect. The structure of the complex was confirmed by single-crystal X-ray diffraction. Transparent PMMA films were fabricated by the drop-casting method changing the amount of complex (1 or 5wt%) and volume of Au NP suspension (10, 20, 50, or 100 µL). The Raman spectra present the PMMA vibrations along with EuIII $^5D_0 \rightarrow {}^7F_{0,1,2}$ luminescence bands. The intensity ratio ($\Delta = IR_{amanl}/I_{lumines}c_{enc}$) of the PMMA vibrational band (2926 cm^{-1}, ν(C–H) stretching) to the EuIIIluminescence (3085 cm^{-1}, $^5D_0 \rightarrow {}^7F_2$ transition) follows an overall trend of increase along with the amount of Au NPs in the films. Yet, when 1% of complex and 20 µL of Au NPs are combined, the intensity ratio falls off the trend and decreases. On the other hand, at 5% complex with 10 µL of Au NPs, Δ has a marked increase. This behavior is associated with a distance-dependent plasmon-enhanced luminescence effect. Thus, the balance between vibrational and luminescence signals in the Raman spectrum can be tuned via the plasmonic influence of Au NPs. The next steps focus on elucidating the luminescence dynamics and assessing the optical thermometry performance.

[1] T. P. Pereira et al. Spectrochim. Acta A 348 (2026) 127177.

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Nanoparticles based on lanthanide–organic frameworks for gas adsorption

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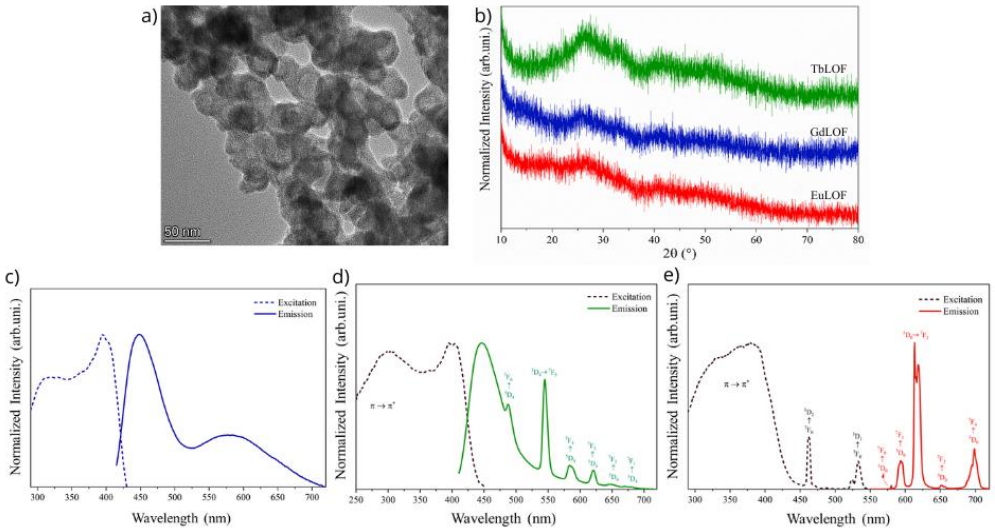
Palavras Chave:*Metal-Organic Framework,Lanthanide,Carbon-dioxide uptake*

Highlights

Three LnLOFs were synthesized by direct precipitation, forming hollow spherical nanoparticles with amorphous structures.
TbLOF is the most promising for CO_2 capture, followed by Gd and EuLOF.

Resumo/Abstract

Porous materials, especially metal-organic frameworks (MOFs), have gained attention in recent years due to their wide range of applications across different fields1–5. When lanthanide ions are used as metal cations, Lanthanide-Organic Frameworks (LOFs) are formed. In this work, three new LnLOFs (Ln = Eu, Gd, and Tb) were synthesized via direct precipitation, and their luminescent properties and CO_2 adsorption were evaluated. TEM revealed the formation of hollow spherical nanoparticles with diameters ranging from 30–50 nm (Figure 1a). The absence of sharp peaks in the diffractograms (Figure 1b) indicates the formation of amorphous materials in all analysed systems. In both GdLOF (Figure 1c) and TbLOF (Figure 1d), the excitation spectrum shows a broad band attributed to ligand absorption. TbLOF emission spectrum shows a broad band with a maximum c.a. 450 nm, assigned to ligand emission, along with narrow bands corresponding to the $^5D_4 \rightarrow {}^7F_j$ (J = 6, 5, 4, 3) transitions typical of Tb^{3+}, with the $^5D_4 \rightarrow {}^7F_5$ transition c.a. 544 nm being the most intense. For EuLOF (Figure 1e), the excitation profile shows a broad band as well as the $^7F_0 \rightarrow {}^5D_2$ and $^7F_0 \rightarrow {}^5D_1$ transitions, indicating that the material can be excited either via the ligand or directly at the Eu^{3+} ion. In the emission spectrum, narrow bands corresponding to the $^5D_0 \rightarrow {}^7FJ$ (J = 0, 1, 2, 3, and 4) transitions characteristic of Eu^{3+} are observed, with the $^5D_0 \rightarrow {}^7F_2$ transition responsible for the red luminescence of the material.CO_2 adsorption measurements indicated that TbLOF is the most promising system (0.13 mmol/g), followed by GdLOF (0.09) and EuLOF (0.06), suggesting that adsorption capacity depends on the size of the lanthanide ion in the framework. Larger ions reduce the adsorption capacity, highlighting the direct influence of LOF composition on the material's adsorptive performance.



a)TEM of EuLOF, b)PXRD of LnLOFs, and excitation/emission spectra of c)GdLOF, d)TbLOF, and e)EuLOF.

Agradecimentos/Acknowledgments

The authors are grateful to the FACEPE, CNPq, CAPES, INCT-LumiNanoTec (408501/2024-3) and FAPESP (2021/08111-2) for the financial support and to the host institutions for their facilities.

New Binuclear Ag(I) Complex Containing Bisphosphine and Substituted Terpyridine: Synthesis, Characterization, and Interaction with Biomolecules.

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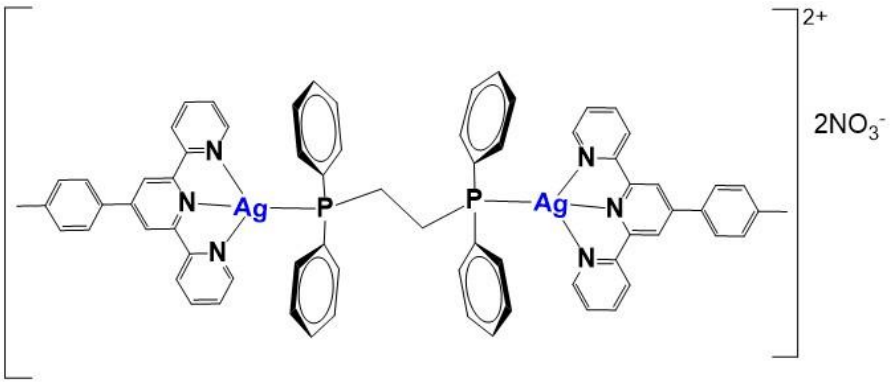
Palavras Chave:*cancer,silver complexes,DNA interaction*

Highlights

Synthesis of a novel binuclear Ag(I) complex containing dppe and MePhTpy. Coordination confirmed by NMR, IR, UV–Vis, and conductivity. Evidence of interaction with DNA via the minor groove.

Resumo/Abstract

Cancer remains one of the leading causes of death worldwide, making it essential to search for more selective chemotherapeutic agents and alternatives to platinum-based drugs. In this context, silver(I) complexes have stood out due to their significant cytotoxic activity and ability to interact with biomolecules through non-covalent pathways. This work reports the synthesis and characterization of a novel binuclear Ag(I) complex containing the 1,2-bis(diphenylphosphine)ethane ligand acting as a bridge and the 4′-(4-Methylphenyl)-2,2′:6′,2″-terpyridine (MePhTpy) ligand. The formation of the complex was confirmed by infrared spectroscopy, which showed characteristic shifts associated with the coordination of the terpyridine ligand to the metal center, as well as the presence of nitrate as a counterion. The ^{1}H and $^{31}P\{^{1}H\}$ NMR spectra, obtained in DMSO-*d6*, showed chemical shifts compatible with the coordination of both bisphosphine and terpyridine to Ag(I), when compared to the spectra of the free ligands. UV-Vis spectroscopy revealed bathochromic shifts of the bands attributed to the dppe ligand, with a shift from 260 nm in the free ligand to 280 nm after coordination, in addition to the appearance of a band at 325 nm, attributed to intraligand transitions involving the coordinated terpyridine. Molar conductivity in DMSO was evaluated as part of the characterization of the complex, and stability studies in DMSO and culture medium at 0, 24, and 48 h indicated that structural integrity was maintained throughout the period analyzed. Preliminary DNA interaction assays, using Hoechst 33258 displacement, showed a decrease in fluorescence intensity, indicating preferential interaction of the complex with DNA through the minor groove. The results presented correspond to an initial stage of the study, which is ongoing, including the expansion of interaction assays with biomolecules and future cellular assays.



Structure of the binuclear Ag(I) complex containing dppe and MePhTpy.

Agradecimentos/Acknowledgments

I would like to thank CAPES, CNPq (305259/2025-3), FAPESP, and the Department of Chemistry at the Federal University of São Carlos (UFSCar) for their institutional support.

New BioMOFs UFMG-1 and UFMG-2 as selective gas sorption platform

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Palavras Chave:*New BioMOFs were prepared from Cu^{2+},piperazine,and oxamidates based on phenylalanine (UFMG-1) and methionine (UFMG-2). UFMG-1 shows high surface area of 971 m^2 g-1,and exceptional H_2/NH_3 adsorption.,BioMOFs*

Highlights

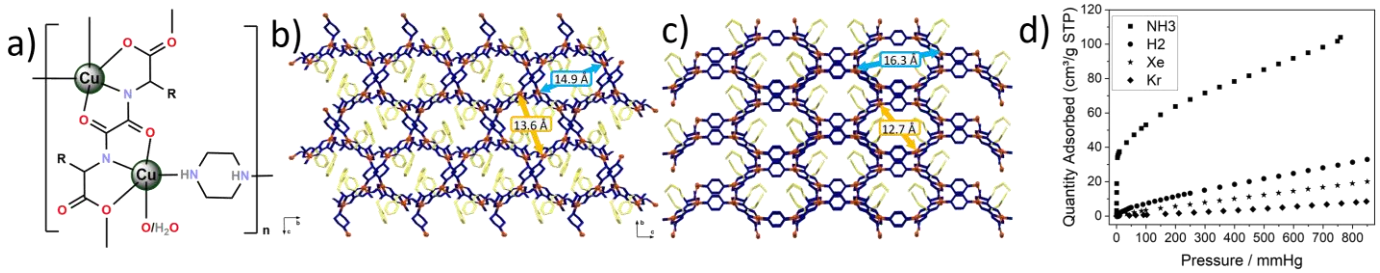
New BioMOFs were prepared from Cu^{2+}, piperazine, and oxamidates based on phenylalanine (**UFMG-1**) and methionine (**UFMG-2**).**UFMG-1**shows high surface area of 971 m^2 g^{-1}, and exceptional H_2/NH_3 adsorption

Resumo/Abstract

MOFs are three-dimensional coordination polymers with potential voids and diverse applications, such as the adsorption of ions and molecules. They can be synthesized with different pore sizes and functional groups oriented toward the pores, allowing the selective entry of species. In this work, we present two new MOFs formed by amino acids (*L*-phenylalanine and*L*-methionine), copper(II) ions, and piperazine, which are biocompatible and of low toxicity, thus classified as BioMOFs. The ligands bis(*N*-phenylalaninate)oxamidate (*L1*) and bis(*N*-methioninate)oxamidate (*L2*) reacted with copper(II) to form complexes with the formula $[Cu_2(L)(H_2O)_4]$. The complexes further reacted with piperazine forming the BioMOFs (Fig. 1a) as blue crystals. The BioMOF synthesized from*L1*is**UFMG-1**, and that from*L2*is**UFMG-2**.

In both BioMOFs,*L1*and*L2*coordinate to two copper atoms in a bis-tridentate fashion, through both carboxylate and amidate groups. A piperazine molecule extends the structure by coordinating to two bimetallic units. To reach a three-dimensional network, in**UFMG-1**, one of the carboxylate groups acts as a μ-*syn-anti*-carboxylate bridge, whereas in**UFMG-2**both carboxylates form this type of bridge. As a result, the copper atoms present a CuN_2O_3 square-pyramidal geometry. In**UFMG-1**, one of the copper atoms have a coordinated water molecule. The BioMOFs exhibit pores along the crystallographic*a*axis (Fig. 1b and 1c), of irregular hexagonal shape, where the amino acid residues reside. For**UFMG-1**the potential pore dimensions are 14.92×13.65 Å² and 16.35×12.66 Å² for**UFMG-2**.

UFMG-1was subjected to gas sorption studies. Its surface area was calculated from CO_2 sorption (273 K, BET method) yielding a high value of 971 m^2 g^{-1}, even with bulky residues oriented toward the pores. In addition, exceptional adsorption of H_2 and NH_3 is observed (Fig. 1d), since after activation one of the copper(II) atoms becomes unsaturated, promoting both chemisorption and physisorption of these gases.



(a) BioMOF monomer. (b) UFMG-1 and (c) UFMG-2 views along a axis. (d) Gas adsorption for UFMG-1.

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New lanthanide complexes with 2-thiophenecarboxylate as a ligand: modulation of synthetic results through controlled experimental variations

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Palavras Chave:*lanthanides, X-ray diffraction, coordination compounds*

Highlights

New lanthanide(III) complexes with 2-thiophenecarboxylate have been obtained using different synthetic routes. Their potential applications include luminescence and magnetic properties.

Resumo/Abstract

A combinação de ligantes orgânicos com lantanídeos pode levar à obtenção de compostos moleculares multifuncionais, com possíveis aplicações ópticas, magnéticas e catalíticas.[1] Neste trabalho, empregou-se o ligante 2-tiofenocarboxilato (2tca), que pode apresentar diferentes modos de coordenação (monodentado, bidentado ou em ponte, unido diferentes centros metálicos).[2] As metodologias consistiram em sínteses*one-pot*, a partir da reação entre 2tca, 1,10-fenantrolina (phen) e os nitratos dos respectivos lantanídeos (Eu^{3+} (**1a**,**1b**) e Dy^{3+} (**2a, 2b**)) em uma mistura EtOH/H_2O 2:1. As misturas foram mantidas em refluxo. Foram empregadas duas proporções estequiométricas lantanídeo/2tca/phen (1:3:1 e 1:2:1) nos ensaios. Monocristais adequados para difração de raios X por monocristal foram obtidos após evaporação lenta das soluções reacionais após cerca de 15 dias. A análise por difração de raios X por monocristal revelou que a variação das proporções estequiométricas gerou diferentes compostos. Os produtos da síntese na proporção 1:3:1 são isomórficos, cristalizando no sistema triclínico, com grupo espacial P, e consistem em estruturas binucleares isomórficas, de fórmula geral $[Ln_2(2tca)_4(phen)_2(NO_3)_2]$ (**Fig. 1a**) (Ln = Eu^{3+} ou Dy^{3+}. Já os complexos oriundos das sínteses 1:2:1 também são binucleares e isomórficos, mas de fórmula $[Ln_2(2tca)_6(phen)_2]$ (**Fig. 1b**), e cristalizaram no sistema monoclínico, com grupo espacial C2/*c*. No primeiro caso, cada íon lantanídeo é coordenado pelos dois átomos de oxigênio de um dos ligantes 2tca e NO_3^-, pelos átomos de nitrogênio de um coligante phen, e por um dos átomos de oxigênio dos demais ligantes 2tca. Já nos produtos das sínteses 1:2:1, não foram observados ânions nitratos coordenados. Todos os compostos obtidos são neutros. Posteriormente, serão estudadas propriedades luminescentes e magnéticas.

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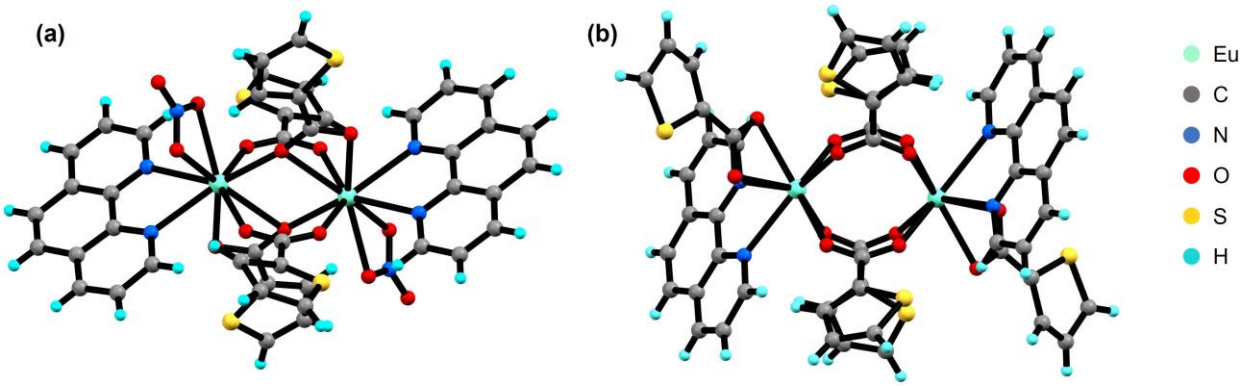


Fig 1. Estruturas cristalinas dos compostos (a) 1a e (b) 1b.

Agradecimentos/Acknowledgments

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On the road to reproducibility: challenges on the multi-step syntesis for obtaining a di-nuclear Zn(II) complex with bis-salodiphen(COOH)4 ligand

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Palavras Chave:*Nitrogenous precursors Bis-salophen binder, Metal complex,Nitrogenous precursors,Bis-salophen binder,Metal complex*

Highlights

The following work presents the experimental optimization study for the preparations of the complex [Zn_2(bis-salophen(COOH)$_4$] and its precursors, for subsequent biological activity analysis.

Resumo/Abstract

This study is focused on the optimization of a multi-step synthesis procedure, involving a series of precursors for the obtention of a zinc(II) di-nuclear complex with a carboxylated-based salophen derivative as ligand. Since the initial planning did not lead to the expected compounds, we investigated potential problems such as reagents purity and synthesis conditions.

To prepare the carboxylated-based salophen derivative, we used the strategy of protecting the 1,2-phenylenediamine with a tosyl group (1st step), followed by nitration with fuming nitric acid on positions 3 and 4 of the benzyl ring (2ⁿd step), deprotection by removing the tosyl group (3rd step), reduction of the nitro group to obtain 1,2,3,4-tetraminobenzene (4th step), and condensation of the latter with 3-formylhydroxybenzoic acid (5th step). For the 1st step, the sample obtained by the reaction between 1,2-phenylendiamine and TsCl in pyridine at 60 °C, followed by the neutralization with HCl solution. ^{1}H NMR spectrum showed that this sample was not the desired product. Thus, we investigated the reagents to improve the synthetic procedure by characterizing and purifying them by recrystallization (1,2-phenylenediamine and TsCl) and distillation under potassium hydroxide (pyridine). In addition we raised the temperature to 100 °C, and the HCl solution was replaced by water. The desired product was then obtained (confirmed by ^{1}HNMR).

For the 3rd step, H_2SO_4 (98 %) was added to a 1,2-dinitro-4,5-bis(p-tosilamino)benzeno sample prepared before the optimization on the 1st step, at 60 °C and kept under constant stirring for four hours. The solution was then poured in cold water giving a pinkish heterogeneous sample with low yield (expected: bordeaux color; 95 % yield).

Although the NMR was consistent with the literature, the aspect and low yield were not indicatives to proceed with the next steps. New experiments are in course from the products obtained after the optimization of the 1st step.

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Pd–Ni Catalyst Derived from Cyanogel: Enhanced Interaction between Metal Elements for Efficient Glycerol Electrooxidation

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Palavras Chave:*glycerol oxidation,renewable energy,hydrogen production*

Highlights

Glycerol oxidation using Pd_2Ni_1 catalyst derived from cyanogel under room temperature Pd_2Ni_1 outperforms segregated Pd–Ni mixtures, delivering higher current density and lower onset potential.

Resumo/Abstract

Nickel–palladium catalysts prepared from cyanogel precursors were explored as electrocatalysts for glycerol oxidation in alkaline medium. The synthetic approach enabled the formation of bimetallic domains with both Pd and Ni atoms in the crystal lattice, contrasting with conventional Pd–Ni mixtures that often display segregated crystal lattices. XRD results showed diffraction peaks located at intermediate 2θ values when compared to those of metallic Ni and Pd with the same crystallographic group (fcc), indicating that cyanogel-derived catalyst exhibited a crystal lattice that incorporated both elements. Structural analysis by SEM showed that the catalysts were formed by porous aggregates, which suggests improved mass transport and availability of active sites. Electrochemical characterization revealed that the Pd_2Ni_1 composition achieved higher current densities and a lower onset potential (100 mV lower) compared to monometallic Pd and a Pd–Ni catalyst derived from non-cyanogel precursors. The enhanced activity was attributed to electronic modifications of Pd sites and optimized active center availability. These findings demonstrate that cyanogel-derived Pd–Ni catalysts represent a promising strategy for biomass valorization and the design of efficient anodic reactions in sustainable energy conversion.

Agradecimentos/Acknowledgments

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Porfirinas e Sn(IV)porfirinas imobilizadas em trititanato de sódio (TNT) e hidróxido duplo lamelar (HDL) para fotodegradação de alaranjado de metila

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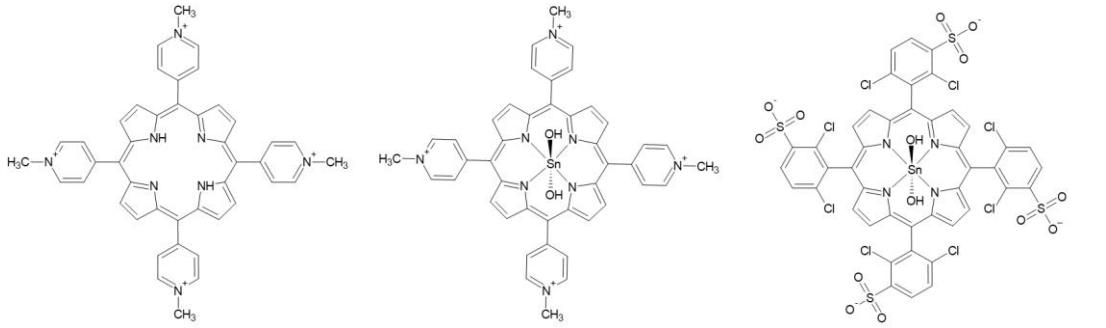
Palavras Chave:*porfirina; fotocatálise; nanotubos de trititanato; hidróxido duplo lamelar,estanho,porfirina,fotocatálise,nanotubos de trititanato,hidróxido duplo lamelar*

Highlights

Sólidos de porfirina/TNT, estanho(IV)porfirina/TNT e estanho(IV)porfirina/HDL avaliados como catalisadores para a degradação de alaranjado de metila sob luz LED.

Resumo/Abstract

Materiais resultantes da imobilização de porfirinas base livre e/ou estanho(IV)porfirina [1] (Fig. 1) em nanotubos de trititanato (TNT) (sólidos [H2P1)]/TNT e [SnP1/TNT) [2] e em hidróxido duplo lamelar de Zn/Al (HDL) (SnP2/HDL) [3] foram preparados e caracterizados (FTIR, UV-Vis e DRX), sugerindo interações predominantemente eletrostáticas/superficiais dos compostos catiônicos H2P1 e SnP1 no TNT e aniônico SnP2 no HDL. Os sólidos foram inicialmente avaliados como catalisadores na degradação do corante alaranjado de metila (AM) sob irradiação luz LED branca (proporção em quantidade de matéria catalisador/AM 1:5, 3 h, 4 lâmpadas de 25 W; 37 °C). A reação controle com TNT não resultou na degradação de AM, enquanto empregando os sólidos H2P1/TNT e SnP1/TNT atingiram cerca de 83% de degradação. No escuro ambos os sólidos não resultaram em degradação evidenciando a participação da luz no processo. Na proporção molar de 1:100 catalisador/corante, o sólido H2P1/TNT promoveu cerca de 55% de degradação, ao passo que SnP1/TNT cerca de 19%, sugerindo influência da metalação, da carga do sensibilizador e/ou de desativação durante a reação. Verificou-se também que empregando-se a H2P1 como catalisador de fase homogênea apenas cerca de 2-4% de degradação do AM foi observada sugerindo o efeito sinergético do suporte TNT no resultado da reação de degradação do AM assistida por luz. Visto ser o sólido de HDL carregado positivamente, foi feito um estudo da adsorção do corante AM nesse suporte onde observou-se uma remoção de 20–54% de AM da solução de reação (dependente da massa de sólido HDL empregada) sendo a cinética de adsorção melhor ajustada para um modelo de pseudo-segunda ordem (R^2=0,9958), indicando quimissorção como etapa limitante. O sólido SnP2/HDL em reações na proporção 1:100 catalisador/AM apresentou cerca de 64% de degradação do AM valor superior ao apresentado pelo HDL puro e pelo processo de adsorção sugerindo algum efeito de degradação do AM empregando esse sólido.



Estrutura de porfirinas e estanho(IV)porfirinas

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Potent cytotoxic effect and high selectivity of a Zn(II) complex against clinically relevant forms of T. cruzi

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Palavras Chave:*Chagas disease,T. cruzi,Zn(II) compound,phendione,in vitro.*

Highlights

A Zn(II) complex presented high cytotoxicity against*T. cruzi,*presenting an IC_{50}value six times lower than benznidazole.

Pharmacokinetic and toxicological parameters were predicted*in silico*.

Resumo/Abstract

Chagas disease is considered a silent disease, given that approximately 95% of infected individuals remain asymptomatic, hindering early diagnosis and effective treatment. The relevance of this approach is reinforced by the fact that, to date, only one drug—benznidazole (BZN)—is available for the treatment of the acute phase of the disease, being ineffective in the chronic phase, which affects most patients.

In this sense, a new Zn(II) compound was synthesized and characterized, presenting the structure: $[Zn(phendione)_3](ClO_4)_2.6H_2O$**(1),**where the Zn(II) center is coordinated to three molecules of the phendione ligand, resulting in a hexacoordinated Zn(II) compound. The structural and compositional characterization of the compound was confirmed by spectroscopic techniques, including ^1H NMR, infrared spectroscopy, and elemental analysis, ensuring the purity and integrity of the obtained structure in DMSO solution.

Compound**1**demonstrated remarkable antiparasitic activity in vitro against trypomastigote forms of*T. cruzi*. The assays indicated a significant reduction in parasite viability from a concentration of 0.1 nM, with the lethal dose 50% (LD_{50}) estimated at 3.2 nM. In comparison, BZN showed an inhibitory effect only from 0.5 µM, with LD_{50} calculated at 1.28 µM. These results demonstrate the superior potency of compound**1**, whose antiparasitic efficacy is in the nanomolar range, in contrast to the micromolar range of BZN. Regarding the intracellular amastigote form, compound**1**exhibited an IC_{50} value of 0.036 µM (36 nM). In turn, the drug BZN exhibited an IC_{50} value of 0.21 µM, representing a potency almost six times lower than that observed for the zinc-based compound. Additionally, some pharmacokinetic and toxicological parameters were predicted*in silico*, showing that this compound exhibits, for example, excellent absorption throughout the gastrointestinal tract after oral administration.

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Central de Análises- Departamento de Química- UFSC.

Preparação e caracterização de sólidos lamelares contendo íons de estanho(IV) para a imobilização de metaloporfirinas e para a investigação catalítica

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Palavras Chave:*Porphyrin,layered double hydroxide,Heterogeneous catalysis,oxidatio*

Highlights

porphrins and metalloporfhyrins immobilized on Zn/Sn/Al layered compounds were synthesized and characterized as robust heterogeneous catalysts for oxidation reactions methylene blue and DHN oxidation

Resumo/Abstract

Porfirinas e as metaloporfirinas (MP) são compostos macrocíclicos muito utilizados como modelos biomiméticos de processos catalíticos de interesse acadêmico e industrial como na fabricação de (foto)catalisadores eficientes e seletivos em reações de oxidação de substratos orgânicos tais como alcanos, corantes, dentre outras. As MP podem ser imobilizadas em diferentes sólidos suporte visando catalisadores mais robustos para processos heterogêneos e reutilizáveis. Como exemplo de suporte temos os sólidos da família dos hidróxidos duplos ou triplos lamelares (HDL), que em geral são formados por metais di e trivalentes ligados por grupos OH-, gerando lamelas positivamente carregadas contendo ânions hidratados entre elas. Neste trabalho, foi preparado dois sólidos lamelares contendo os metais Sn4+/Zn2+ e Al3+/Sn4+/Zn2+ com o objetivo de serem usados como suporte para a imobilização de estanho(IV)porfirinas aniônicas (SnP). Tanto os sólidos lamelares quanto os sólidos contendo SnP foram investigados como catalisadores em diferentes reações de oxidação (por exemplo: degradação do corante azul de metileno (AM) e do DHN (1,5-diidroxinaftaleno). O sólido de Zn2+/Sn4+ (1:3) foi preparado pelo método da precipitação até pH 9,6 a 22 °C empregando sais de SnCl4·5H2O 2,5×10-2 molL-1 e ZnCl2 8,0×10-2 molL-1, além da solução de NaOH 1,0 mol L-1 e de Na2CO3 1,9×10-3 mol L-1. O sólido de composição trimetálica Zn/Al/Sn (3:5:1) também foi preparado pelo método da precipitação até pH 10, empregando as soluções dos sais de Sn4+ 2,0 ×10-3 mol L-1, Zn2+ 0,03 mol L-1 e Al3+ 8,2 ×10-3 mol L-1, além de uma solução de NaOH 0,06 mol L -1 e de Na2CO3 0,02 mol L-1, a 26 °C com agitação constante. Os sólidos obtidos foram caracterizados por MEV, DRX e FTIR. Testes catalíticos com os HDL mostraram em média 82% de degradação do AM quando a reação ocorreu na presença de luz branca de led. Na oxidação do DHN o sólido de HDL bimetálico apresentou a conversão de 10,76% a juglona.

Agradecimentos/Acknowledgments

CAPES, CNPq, Fundação Araucária e Instituto Nacional de Ciência e Tecnologia em Ciências Moleculares (INCT-CiMol), Projeto CNPq 406804/2022-2

Primary Coordination Sphere Effects on the Reactivity of Nitrosylsulphito Complexes

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Palavras Chave:*Ruthenium complexes,Nitrosylsulphito,Ligand effects,structure–reactivity,Photochemistry*

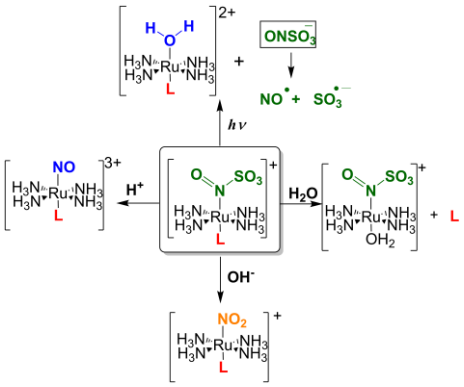
Highlights

-Ligand basicity governs the reactivity of Ru nitrosylsulphito complexes-

-Hydroxide reactivity confirms the nucleophilic character of N(O)SO3-
-Photolysis generates NO• and SO3-• radicals

Resumo/Abstract

This work describes the reactivity of ruthenium nitrosylsulphito complexes of the general formula trans-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$ where L are the N-heterocyclic ligands: pyrazine (pz), isonicotinamide (isn), isonicotinic acid (ina), pyridine (py) or 4-picoline. The ligand L positioned trans to $N(O)SO_3^-$ strongly influences the stability and reactivity of these complexes. Ligand L labilization rate constant in aqueous solution (pH 7.4, 25°C) follow the order, pz>isn>ina>py>4-pic. The rate constants varying from k = 3.40 x 10–⁴ s–¹ ($t_1/_2$ = 34 min) for L = pz to 1.7 x 10^{-6} s^{-1} ($t_1/_2$ = 6800 min = 113h) for L = 4-pic. A linear correlation was observed between the -log k (pk) and the pK_a values of the conjugated acids of the ligands (pKaH), with R2 ~ 0.97, demonstrating that ligand basicity governs the lability of L and enables prediction of complex stability in aqueous media. The pK_a of the $-SO_3$ moiety of the coordinated $N(O)SO_3^-$ ligand was determined at 25°C, ranging from 4.6 (L = pz) to 5.6 (L = py). Reaction of trans-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$ with hydroxide ions (OH^-) yielded the corresponding nitro complexes trans-$[Ru(NH_3)_4(L)(NO_2)]^+$, with rate constants between k = 5.2 and 8.5 $M^{-1}s^{-1}$, indicating minimal influence of L on this reaction, and confirming the nucleophilic character of the $N(O)SO_3^-$ nitrogen. All trans-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$ showed a characteristic metal-to-ligand charge-transfer transition (MLCT, Ru→$NOSO_3$) at λ_{max} = 358-369 nm. A linear correlation (R^2 = 0.99) was found between the MLCT transition energy (cm-1) and the pK_aH of L. Photolysis of trans-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$ induced labilization of $N(O)SO_3^-$ ligand, which is unstable at room temperature, leading to cleavage of the N–S bond and generation of the radicals NO• and $SO_3^{\bullet -}$. Overall, these results demonstrate that the reactivity and physicochemical properties of trans-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$ complexes can be systematically tuned and predicted based on the basicity of the ligand trans to $N(O)SO_3^-$.



Summary of the reactivity of trans-[Ru(NH3)4(L)(N(O)SO3)]+ complexes

Agradecimentos/Acknowledgments

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Ratiometric thermometry combining luminescence and Raman bands in PMMA films containing a EuIII β-diketonate complex

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Palavras Chave:*Lanthanides,Rare earths,Sensors,Luminescence,Coordination chemistry*

Highlights

Dispersion of EuIIIcomplexes in PMMA enables the detection of PMMA vibrations and EuIII luminescence in the Raman spectrum;

Optical ratiometric thermometry combining Raman and luminescence bands.

Resumo/Abstract

Optical thermometry plays a key role in measuring the temperature at the nanoscale in chemical or biological processes. Raman and luminescence thermography are among the most used techniques employed for that. However, Raman thermometry still presents limited thermal sensitivity while luminescence thermometry depends on combined factors such as brightness and temperature dependence of luminescence following well-known models. To take advantage of the maximum potential of both techniques, herein, we report the combination of Raman and luminescence bands measured in a single Raman spectrum to calculate a ratiometric thermometric parameter ($\Delta = I_l u_m i_{ne_s} c_{e_n} c_e / IR_{a_m a_n}$). For that, the red-emitting $[Eu(nta)_3(phen)]$ (nta = 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione; phen = 1,10-phenanthroline) complex was dispersed in poly(methyl methacrylate) (PMMA) seeking to combine the vibrational Raman bands of the PMMA polymer and the EuIII luminescence in the complex. The synthesized films by the drop casting method (1wt% of complex to PMMA) are transparent, thermally stable up to 450 K, and present a homogeneous surface. Temperature-dependent Raman spectrum (100 to 420 K) indicates that the ratio of the PMMA vibrational band (ν(C-H)) to the EuIIIluminescence ($^5D_0 \rightarrow {}^7F_2$ transition) presents a strong dependence on the temperature. Below 280 K, Raman-dominated exponential response is observed (maximum relative thermal sensitivity, S_m, of 1.1% K^{-1} at 280 K), while up this temperature, a luminescence-driven response takes place (S_m of 5.2% K^{-1} at 420 K). Looking for repeatability, nine heating–cooling cycles (100 – 420 K) were undertaken, and the thermometric parameter remained unchanged, confirming the robustness of the technique. Thus, the ratiometric approach based on luminescence and Raman bands is a versatile approach for designing sensitive temperature probes with temperature monitoring flexibility.[1]
[1] T. P. Pereira et al. Spectrochim. Acta A 348 (2026) 127177.

Agradecimentos/Acknowledgments

To FAPESP for the scholarship provided for TPP (2025/04765-9). AGBJ thanks the Support Program for New Faculty at USP from PRPI - USP.

Síntese, caracterização espectroscópica e propriedades de um complexo de cobre tetrazólico

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Palavras Chave:*Química de coordenação,Complexos metálicos,Tetrazol,Cobre*

Highlights

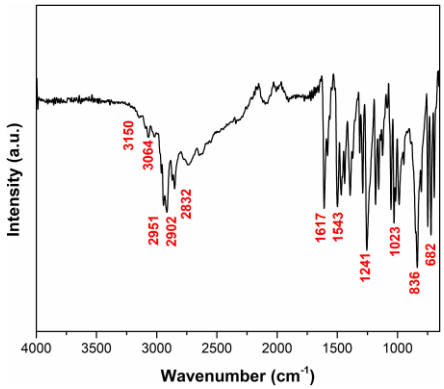
Synthesis, spectroscopic characterization and physicochemical properties of a copper tetrazole complex.

Resumo/Abstract

A química de coordenação desempenha papel central no desenvolvimento de complexos metálicos com propriedades estruturais e físico-químicas relevantes. Ligantes derivados de tetrazol destacam-se pela elevada densidade eletrônica e versatilidade de coordenação, favorecendo a formação de complexos estáveis com metais de transição. Nesse contexto, este trabalho teve como objetivo a síntese, caracterização espectroscópica e investigação das propriedades de um complexo de cobre contendo ligante tetrazólico.

O complexo foi obtido por reação em meio etanólico entre $Cu(NO_3)_2 \cdot 3H_2O$ e ligantes orgânicos, sob agitação constante por 48 h a 50 °C, sendo isolado como sólido cristalino após filtração e lavagem com acetonitrila. A caracterização envolveu testes de solubilidade, determinação da temperatura de decomposição, medidas de condutividade eletrolítica, espectroscopia de infravermelho, microscopia eletrônica de varredura (MEV), espectroscopia de raios X por dispersão em energia (EDS) e análise textural por adsorção/dessorção de N_2.

O complexo apresentou solubilidade em DMSO, DMF e acetonitrila, sendo insolúvel em água e solventes menos polares, além de decomposição térmica a 210 °C. A condutividade em DMSO (50,31 $\mu S \cdot cm^{-1}$) indicou comportamento de eletrólito fraco. A espectroscopia de infravermelho evidenciou bandas características do ligante tetrazólico, Figura 1, destacando-se vibrações associadas aos grupos C=N e N=N e a presença da banda em 682 cm^{-1} atribuída à vibração ν(Cu–N), confirmando a coordenação do ligante ao centro metálico. A análise por MEV revelou morfologia homogênea do sólido, enquanto a microanálise por EDS confirmou a composição elementar do complexo. A análise textural indicou comportamento mesoporoso, com área superficial específica de 152,4 $m^2 \cdot g^{-1}$, volume total de poros de 0,312 $cm^3 \cdot g^{-1}$ e diâmetro médio de 8,2 nm. Os resultados contribuem para o entendimento das propriedades espectroscópicas e físico-químicas de complexos de cobre tetrazólicos.



Espectro de FTIR com bandas características do complexo de cobre.

Agradecimentos/Acknowledgments

A Universidade Federal de Roraima (UFRR) e Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

Síntese de dímeros homo e heteronucleares de Nd^{3+} e Yb^{3+} para o estudo da transferência de energia e luminescência via mecanismo de downshifting.

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Palavras Chave:*lantanídeos, luminescência, difração de raios X, complexos metálicos, downshifting*

Highlights

Complexos dinucleares de Yb^{3+} e Nd^{3+} foram sintetizados com $acac^-$ e dppeo. Os dados ópticos mostram emissão em ~980 nm e evidenciam emissão downshifting via transferência $Nd^{3+} \rightarrow Yb^{3+}$.

Resumo/Abstract

Complexos luminescentes à base de íons lantanídeos (Ln^{3+}) têm sido amplamente estudados devido às suas características fotofísicas e à eficiência dos processos de transferência de energia associados ao mecanismo de downshifting. Esse mecanismo é de grande importância por permitir a conversão de radiação de absorção de alta energia em uma emissão de menor energia, com aplicações em dispositivos fotônicos e sensores luminescentes. Assim, este trabalho propõe a obtenção de dímeros homo e heteronucleares à base de Yb^{3+} e Nd^{3+}, utilizando o acetilacetonato (acac-) como ligante terminal e o (difenil)bisfosfinóxido (dppeo) como ligante em ponte, visando à investigação dos processos de transferência de energia entre os centros metálicos e à elucidação do mecanismo de downshifting nesses sistemas. Para isso, uma solução etanólica de dppeo foi adicionada à solução contendo o sal de lantanídeo, seguida da adição de uma solução etanólica de acac–, resultando nas estruturas $[YbNd(acac)_6(H_2O)_2(\mu\text{-dppeo})]$ e $[Yb_2(acac)_6(H_2O)_2(\mu\text{-dppeo})]$, as quais foram caracterizadas pelas técnicas de difração de raios X em pó (DRX), espectroscopia de fotoluminescência e espectroscopia no infravermelho (FTIR). Os espectros FTIR mostram que os produtos finais apresentam estiramentos C=O (1580–1600 cm^{-1}) e P=O (1171 cm^{-1}) deslocados para menores números de onda em comparação aos ligantes precursores isolados, sugerindo a coordenação ao centro metálico. Os compostos foram analisados por espectroscopia de fotoluminescência, e em ambos os sistemas investigados, observa-se exclusivamente a emissão característica do Yb^{3+} em aproximadamente 980 nm, atribuída a transição intraconfiguracional $^2F_{5,2} \rightarrow {}^2F_{7,2}$. A ausência das bandas emissivas do Nd^{3+} no composto $[YbNd(acac)_6(H_2O)_2(\mu\text{-dppeo})]$ pode indicar uma transferência do Nd^{3+} para o Yb^{3+} a partir do nível $^4F_{3/2}$, o que resultou em uma supressão da emissão radiativa do Nd^{3+} e na atuação do Yb^{3+} como centro emissor final do processo de downshifting.

Agradecimentos/Acknowledgments

Os autores agradecem a CNPq, FAPESP, CAPES e LumiNanoTech

Síntese e caracterização de novos nitrosilo-complexos de Rutênio(II) com o ligante 4,5-diazafluoren-9-ona

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Palavras Chave:*Nitrosilo-complexos,Rutênio,Doadores de NO*

Highlights

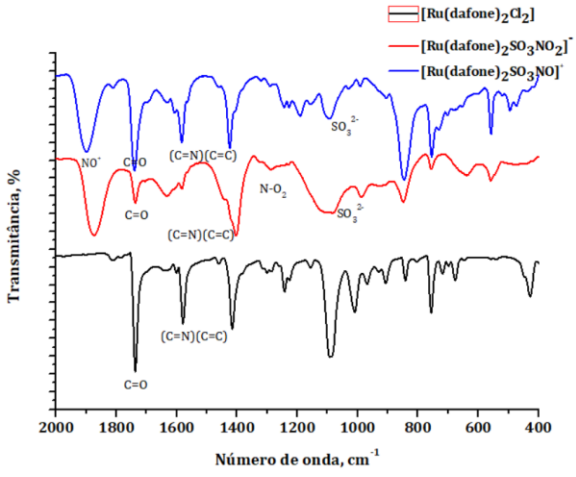
Synthesis of new Ru-nitrosyl complexes with 4,5-diazafluoren-9-ona.

Linear NO coordination confirmed by IR (1.904 cm-1).

Potential nitric oxide donos for therapeutic applications.

Resumo/Abstract

O óxido nítrico (NO) desempenha funções biológicas importantes, tornando complexos de rutênio doadores de NO promissores para terapias cardiovasculares e antitumorais. Este trabalho descreve a síntese e a caracterização dos complexos $[Ru(dafone)_2Cl_2]$ (1), $[Ru(dafone)2(SO_3)(NO_2)]^-$ (2) e $[Ru(dafone)_2SO_3NO]^+$ (3) (dafone=4,5-diazafluoren-9-ona). O ligante dafone foi escolhido devido a sua versatilidade eletrônica e potencial atividade citotóxica. O precursor 1 foi obtido via reação do*cis*-$[RuCl_2(DMSO)_4]$ com dafone (1:2) em etanol sob refluxo por 5h em atmosfera de argônio. O complexo 2 foi sintetizado por reação com Na_2SO_3 e posterior adição de $NaNO_2$ em mistura $EtOH/H_2O$ (1:1) sob refluxo, sendo sua formação confirmada via espectroscopia vibracional na região do infravermelho (IV), apresentando estiramentos característicos do grupo nitro (ν_{ass}= 1.328 cm^{-1} e ν_s = 1.292 cm^{-1}) e bandas do grupo sulfito em 1.111 e 1.079 cm^{-1} (S-coordenado). O complexo 3 foi sintetizado pela reação do intermediário com CF_3COOH em metanol, sendo precipitado como sal de NH_4PF_6. No IV do complexo precursor revelou o estiramento ν(C=O) em 1.731 cm^{-1}, enquanto o complexo 3 apresentou uma banda diagnóstica intensa em 1.904 cm^{-1}, confirmando a coordenação linear do ligante nitrosilo na forma de NO^+. Na espectroscopia eletrônica de absorção na região do ultravioleta-visível (UV-Vis) em $CHCl_3$, a banda de transferência de carga metal-ligante (MLCT) de 1 (450 nm) sofreu deslocamento hipsocrômico para 415 nm em 3. Este deslocamento de 35 nm reflete a forte estabilização dos orbitais dπ do centro metálico pelo caráter aceptor-π do NO^+. Os resultados preliminares fornecem evidencias da formação de novos sistemas $\{RuNO\}^6$ lineares, sobre os quais estudos complementares de caracterização e reatividade encontram-se atualmente em desenvolvimento.



Espectros vibracionais na região do infravermelho (IV) dos complexos (1), (2) e (3).

Agradecimentos/Acknowledgments

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Síntese e caracterização de uma nova hidrazona contendo morfolina e seu complexo de zinco(II) para aplicações medicinais com atividade desfosforilante

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Palavras Chave:*N-acil-hidrazonas, complexo de zinco(II), síntese, caracterização,N-acil-hidrazonas,complexo de zinco(II),síntese,caracterização*

Highlights

A new hydrazone containing 1-methylimidazole and morpholine, as well as its zinc(II) complex, were synthesized and characterized and will be evaluated for their protein dephosphorylation capabilities.

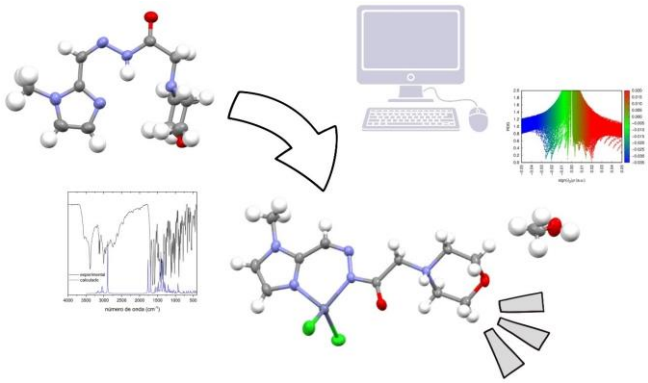
Resumo/Abstract

N-acil-hidrazonas e seus complexos têm sido muito investigados em razão de suas atividades biológicas e aplicações farmacológicas.[1] A seleção de substratos já empregados na indústria farmacêutica facilita o planejamento racional de novos candidatos a fármacos. A morfolina e o anel imidazólico, bem como seus derivados, apresentam elevada biocompatibilidade, sendo amplamente empregados na indústria farmacêutica.[2,3] Neste contexto, a 2-morfolina acetohidrazida e o 1-metilimidazol-2-carboxaldeído foram selecionados como precursores para a síntese de um ligante hidrazônico inédito.**X1MPH**foi sintetizado a partir de uma reação de condensação e obtido na forma de monocristais, caracterizados por difração de raios-X, infravermelho médio, termogravimetria e ressonância magnética nuclear de ^{1}H. O complexo**Zn(X1MPH)**, por sua vez, foi preparado pela reação entre o ligante e $ZnCl_2$ e obtido também como monocristais que foram estruturalmente caracterizados. O**X1MPH**apresentou uma conformação estrutural inesperada, onde o grupo NH encontra-se em conformação*anti*em relação à carbonila e*syn*em relação ao anel morfolínico. Esse arranjo tridimensional pôde ser explicado pela presença de uma interação intramolecular de hidrogênio bifurcada, na qual o NH hidrazônico atua como doador de hidrogênio para $N_mid_aZ_{ol}$ e $N_morf_{ol}i_na$. Cálculos teóricos demonstraram que essa interação de hidrogênio confere uma estabilidade de –3,6 kcal mol–^{1}. Em**Zn(X1MPH)**observa-se a amida desprotonada e o ligante coordenando através do $N_am id_a$ e $Ni_mid_aZ_{ol}$, enquanto o $N_morf_{ol}i_na$está protonado, em uma tautomeria induzida pela coordenação. Por fim, 2 cloretos completam a esfera de coordenação tetraédrica do metal. Espera-se que esses sítios lábeis sejam capazes de conferir atividade desfosforilante à espécie, o que será avaliado futuramente através de ensaios*in vitro*.

1 HAMZI, I. Mini-Rev Org Chem, 19(8), 2022, 968-990

2 KUMARI,A; SINGH, R. K. Bioorg Chem, 96, 2020

3 RANI, N; SINGH, R; KUMAR, P. Curr Org Synth. 2023



Nova hidrazona contendo morfolina e seu complexo de zinco(II) para aplicações medicinais

Agradecimentos/Acknowledgments

PIBIC UERJ, CAPES, FAPERJ

Síntese e Caracterização de um Novo Complexo Porfirínico de Ag(I) com o Ligante 4'-(4-Metilfenil)-2,2':6',2''-terpiridina.

Karol Keilla Franzoni (IC)*[1], Nádija Natalice Paixão da Silva (PG)[2], Fillipe Vieira Rocha (PQ)[1].

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Palavras Chave:*Complexos de Prata; Terapia Fotodinâmica; Porfirina*

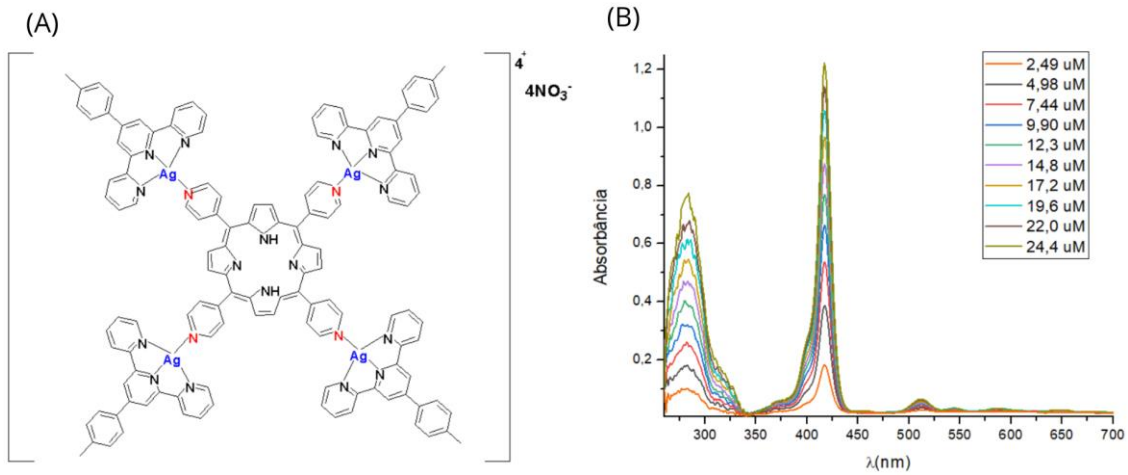
Highlights

"Synthesis of a tetracoordinate porphyrinic complex in the periphery containing silver and terpyridine ligand"

"Spectroscopic characterization via ^{1}H NMR, UV-vis, infrared"

Resumo/Abstract

O câncer está entre as principais causas de morte no mundo, apresentando um aumento crescente de sua incidência ao longo dos anos. Diante desse cenário, diversos tratamentos têm sido desenvolvidos a fim de combater a doença, no entanto, os métodos convencionais causam efeitos colaterais, comprometendo a saúde do paciente. Nesse âmbito, a Terapia Fotodinâmica (TFD) tem se tornado destaque pelo uso de abordagem minimamente invasiva, baseada na interação entre um fotossensibilizador e luz em um comprimento de onda adequado, o qual ativa as propriedades citotóxicas da molécula. Essa combinação promove a geração de espécies reativas de oxigênio e ou oxigênio singlet capazes de induzir morte celular, potencializando a eficácia do tratamento e minimizando os danos aos tecidos saudáveis. Com base nisso, o objetivo desta pesquisa é desenvolver um novo complexo porfirínico (5,10,15,20-Tetra(4-piridil)-21H,23H-porfirina) tetra coordenado de prata (I) com ligante terpiridínico (4'-(4-Metilfenil)-2,2':6',2''-terpiridina) que possa atuar como fotossensibilizante. O complexo sintetizado foi caracterizado pelas técnicas de ressonância magnética nuclear (^{1}H e COSY), condutividade molar, espectroscopia de absorção na região do infravermelho (IV) e na região do ultravioleta-visível (UV-Vis), espectrometria de massas. Os resultados obtidos de espectroscopia de absorção na região do ultravioleta-visível apresentaram bandas características dos compostos coordenados. A porfirina, revelou a banda Soret em 417 nm, e as bandas Q em 512 nm, 545 nm, 585 nm e 648 nm do macrociclo tetrapirrólico; a terpiridina evidenciou as bandas em 283 nm e 320 nm, sendo característica do composto. Ademais, pelo espectro de RMN de ^{1}H foi possível constatar a razão estequiométrica esperada entre o ligante terperidínico e a porfirina em uma razão 1:4, respectivamente. Tais resultados são indícios da coordenação da porfirina ao centro metálico.



(A) Proposta estrutural do complexo. (B) Espectro de Uv-vis do complexo.

Agradecimentos/Acknowledgments

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Síntese e estudo de propriedades luminescentes de [Ln(OAc)(tta)2]n e aplicação em filme polimérico para modulação de luz

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Palavras Chave:*polímeros de coordenação, lantanídeos, modulação espectral*

Highlights

Os compostos $[Ln(OAc)(tta)_2]_n$(Ln = Eu^{3+}, Gd^{3+}, Tb^{3+}) foram sintetizados e suas propriedades luminescentes determinadas. O derivado de Eu^{3+} foi impregnado em filme polimérico para modulação espectral.

Resumo/Abstract

A modulação espectral da radiação solar por meio de materiais fotoluminescentes constitui uma estratégia eficiente para o controle da luz incidente, permitindo conversão de faixas espectrais menos desejáveis em faixas de maior interesse, por exemplo no uso em estufas. Nesse contexto, compostos capazes de absorver radiação ultravioleta (UV, 200–400 nm) e reemitir no visível (400–750 nm) destacam-se como sistemas promissores para aplicações em materiais ópticos. Os íons lantanídeos (Ln^{3+}) são adequados para esse propósito devido às transições intraconfiguracionais 4*f*–4*f*, que resultam em emissões estreitas e bem definidas. Dentre eles, Eu^{3+} e Tb^{3+} apresentam emissões intensas nas regiões do vermelho e do verde, respectivamente. A eficiência das emissões está diretamente relacionada ao efeito antena promovido por ligantes orgânicos, que comumente absorvem radiação UV e transferem energia para o centro emissor. Neste trabalho, são investigados os polímeros de coordenação $[Ln(OAc)(tta)_2]_n$(Ln = Eu^{3+}, Gd^{3+}, Tb^{3+}; tta = 2-tenoiltrifluoroacetona). O análogo contendo Gd^{3+}, íon inativo na região do visível, é empregado como sistema de referência para a elucidação das propriedades eletrônicas do ligante, permitindo avaliar processos de absorção, transferência de energia e perdas não radiativas. Os compostos foram obtidos na forma cristalina com rendimentos de reação entre 59–70%. Todos os compostos foram caracterizados por técnicas espectroscópicas (FTIR, excitação/emissão, rendimento quântico, tempo de vida), difração de raios X em monocristal e termogravimetria. A impregnação do composto $[Eu(OAc)(tta)_2]_n$em filme polimérico de EVA (etileno e acetato de vinila) resulta em um aumento do rendimento quântico de emissão, atribuído à maior rigidez do ambiente e à redução de processos de desativação não radiativa, comprovando o potencial desse sistema para o desenvolvimento de materiais luminescentes avançados.

Agradecimentos/Acknowledgments

Os autores agradecem à FAPESP, CNPq, CAPES e Braskem.

Solvent effect on cyclohexane hydroxylation catalyzed by cationic Mn porphyrins heterogenized on silica gel

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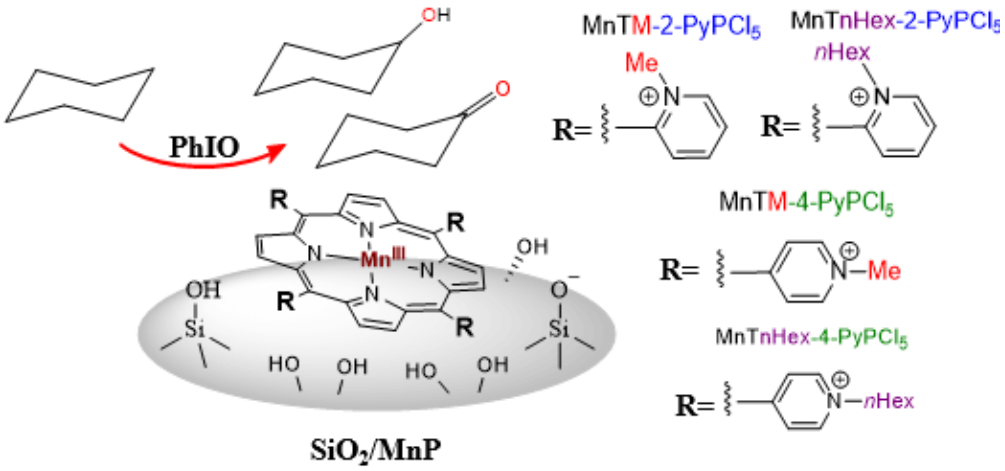
Palavras Chave:*Immobilized Mn-porphyrins, oxidation catalysts, biomimetic catalysis, solvent polarity, selectivity.*

Highlights

Using cyclohexane hydroxylation as model reaction, cationic Mn porphyrins immobilized onto SiO_2 showed catalytic efficiency modulated by solvent polarity; cyclohexanol selectivity was little affected.

Resumo/Abstract

The selective hydroxylation of alkanes to alcohols under mild conditions remains a major challenge in catalysis, since sequential oxidation to ketones is favored. Mn(III) porphyrins (MnPs) are effective biomimetic models of cytochromes P450 for alkane hydroxylation. MnP application in homogeneous catalysis is often limited by susceptibility to oxidative degradation and difficulties in MnP recovery, which justifies MnP immobilization on inert supports for use in heterogenous catalysis. In this work, solvent, MnP isomer, and MnP alkyl side-chain effects on the cyclohexane hydroxylation catalyzed by MnPs supported on chromatographic silica gel were investigated. Four materials derived from the electrostatic heterogenization of Mn(III)*N*-alkylpyridylporphyrins on SiO_2 were evaluated: the*ortho*isomers (MnTalkyl-2-PyP^{5+}; alkyl = Me or*n*Hex) and*para*isomers (MnTalkyl-4-PyP^{5+}; alkyl = Me or*n*Hex). The reactions were carried out in MeCN (polar solvent), $CHCl_3$ (low-polarity solvent) or the binary $CHCl_3$:MeCN (1:1, v/v) mixture. In MeCN, the SiO_2/MnTnHex-4-PyPCl_5 catalyst showed the highest efficiency (98%). In $CHCl_3$, the efficiency of this catalyst also stood out (73%), as the efficiencies for the other SiO_2/MnP systems ranged from 52–61%. Remarkably, in the binary mixture, the SiO_2/MnPs systems were less efficient than in the pure solvents; with exception of SiO_2/MnTnHex-4-PyPCl_5 that showed yields closer to those in $CHCl_3$. Whereas the solvent impacted significantly catalyst efficiency, it had little effect on selectivity. Selectivity was, however, dependent on MnP isomer: irrespective of the solvent, the*ortho*MnPs (SiO_2/MnTalkyl-2-PyPCl_5) exhibited higher selectivities than those of the corresponding*para*isomers (SiO_2/MnTalkyl-4-PyPCl_5). An attempted modeling of the structure-property relationships on these SiO_2/MnP-based systems was carried out by chemometric analyses.



Representation of cyclohexane hydroxylation catalyzed by SiO_2/MnP

Agradecimentos/Acknowledgments

CNPq, CAPES, FINEP, INCT-CiMol

Spectroscopic Study of Color Center Formation in Pr3+/Eu3+ Doped Fluorophosphate Glasses

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Palavras Chave:*luminescence thermometry, rare earth, phosphate glasses,Color Centers,Luminescence Thermometry,Rare Earth,Phosphate Glasses*

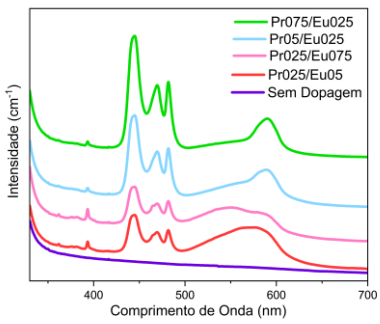
Highlights

Thermally induced P-OHC color center formation in phosphate glasses. Pr3+/Eu3+ synergy for ratiometric luminescence thermometry. Rare earth ions reduction induced chromatic shifts.

Resumo/Abstract

The combination of**rare-earth (RE) ions**with glass matrices allows for the exploration of narrow energy levels within a material that is both mechanically robust and stable against degradation. One of the most investigated applications involving rare earths and sensing is**luminescence thermometry**. This technique utilizes ratiometric variations in emission spectra, excitation, and lifetimes to remotely determine the temperature of a system. Parallel to this, a recurring but understudied phenomenon in rare-earth-doped phosphate glasses is the significant**chromatic change**observed after thermal treatment.
This work seeks to understand the origin of these color variations while performing the synthesis and characterization of oxyfluoride glasses co-doped with varying proportions of Pr^{3+} and Eu^{3+} for applications in luminescence temperature sensing.
One of the potential causes attributed to this effect is the formation of**color centers**, specifically**P-OHC (Phosphorus Oxygen Hole Centers)**. These are defects in which the chemical bonding structure of the material is altered. These changes occur due to**charge transfers**between rare earths with higher reduction potential (such as Eu^{3+}, Yb^{3+}, and Sm^{3+}) and non-bridging oxygens (NBOs) bonded to phosphorus atoms.

Figure 1 presents the UV-Vis absorption spectra, identifying the characteristic**absorption bands**of Pr^{3+} and Eu^{3+}, whose intensities and ratios increase with concentration. As is typical for rare-earth ions, the absorption features narrow bands corresponding to transitions between**f-sublevels**, enabling the selective excitation of different ions within the same material. The**spectral signature**of the color centers is also observed as a broad band centered between 500 and 600 nm. There is a noticeable broadening and increase in band intensity as the proportion of europium dopant increases, likely originating from energy transfer between the europium and oxygen.



UV-Vis absorption spectra of doped Pr3+/Eu3+ glasses.

Agradecimentos/Acknowledgments

This work is supported by the**University of São Paulo (USP)**, the**São Carlos Institute of Chemistry (IQSC)**, and the**São Paulo Research Foundation (FAPESP)**, grant number 2025/03704-6.

Stoichiometry-Driven Modulation of Magnetic Anisotropy in Mononuclear Cu(II) Complexes: An EPR and Computational Study

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Palavras Chave:*quinoline,easy plane complex,easy axis complex,Magnetism,g Tensor*

Highlights

New mononuclear Cu(II) complexes reported. Reaction stoichiometry tunes Magnetic Anisotropy. EPR reveals easy-plane and easy-axis behavior.*g*-Tensor anisotropy supported by theory.

Resumo/Abstract

Mononuclear Cu(II) complexes are relevant model systems for investigating magnetic anisotropy and spin-orbit coupling by Electron Paramagnetic Resonance (EPR) spectroscopy.[1,2]This work reports experimental and computational studies of complexes**PB3**and**PB4**, obtained from the ethyl alpha-(quinolin-8-ylamino) acrylate proligand (**1**) using metal-to-ligand ratios of 1:1 and 1:2, respectively. Magnetic properties were investigated by EPR in the solid state (polycrystalline samples) and in solution at 50 and 10 K. In the solid state, both complexes display anisotropic EPR spectra typical of Cu(II) centers (S = 1/2), indicating axially distorted electronic environments.**PB3**exhibits easy-plane behavior, with the largest*g*component associated with the plane perpendicular to the*z*axis, whereas**PB4**shows easy-axis behavior with pronounced axial anisotropy. In solution, a marked improvement in spectral resolution is observed for both complexes, with well-resolved hyperfine lines arising from the interaction between the electronic spin and the cupper nucleus (I = 3/2), attributed to increased molecular mobility and reduced line broadening. For**PB3**, the hyperfine structure is mainly observed in the region associated with*g*perpendicular, while for**PB4**the spectra suggest a reorganization of the axis associated with the largest*g*value. Theoretical calculations for the prediction of*g*tensors show excellent agreement with the experimental data, supporting the spectral assignments and highlighting the role of spin-orbit coupling and crystal field distortion. Overall, the results demonstrate that changes in metal-to-ligand stoichiometry significantly modulate the magnetic anisotropy of mononuclear Cu(II) complexes.

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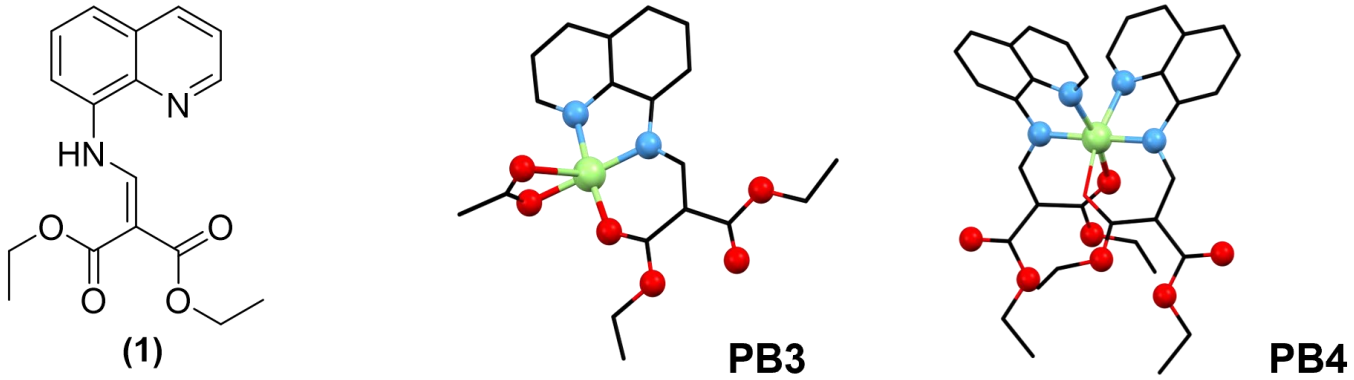


Figure 1. Pro-ligand 1, PB3 complex with 1:1 stoichiometry and PB4 complex with 2:1 stoichiometry.

Agradecimentos/Acknowledgments

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Structural Insights and Anticancer Activity of Newly Synthesized Gold(I) Dithiocarbamate Complexes

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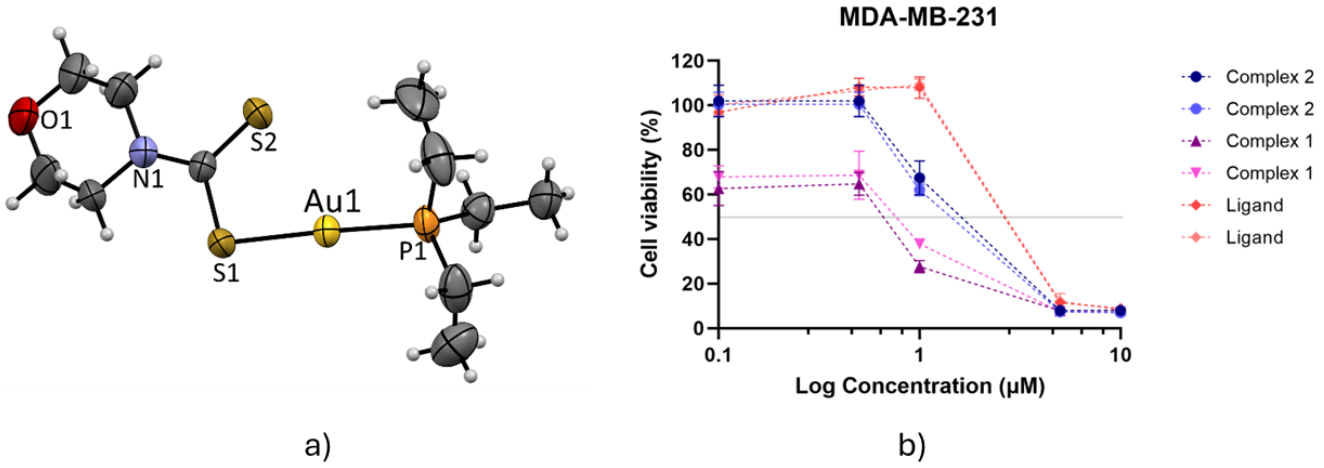
Palavras Chave:*Methalodrugs,Antitumor,X-Ray Diffraction,Cytotoxicity*

Highlights

New gold(I) dithiocarbamate complexes were characterized by NMR and XRD and revealed promising anticancer activity in breast and lung cancer cell lines.

Resumo/Abstract

Gold complexes with organosulfur ligands, such as dithiocarbamates, have shown promising potential due to their anticancer activity and the presence of the Au–S bond, which may alternatively help overcome the adverse effects caused by platinum complexes. In this context, this work aims at the synthesis, characterization, and investigation of the antitumor activity of new gold(I) complexes bearing dithiocarbamate ligands. The complexes were synthesized in a 1:1 reaction between the gold precursors PR_3AuCl (1: R = Et; 2: R = Ph) and the morpholine-derived dithiocarbamate ligand in a solvent mixture under stirring for 30 min to 1 h. The products were obtained by solvent evaporation and were properly characterized by NMR spectroscopy. Complex 1 was recrystallized by slow evaporation, and its structure was confirmed by single-crystal X-ray diffraction. The in vitro cytotoxicity assay was performed against MDA-MB-231 and A549 cancer cell lines. Crystal structure of complex 1 confirms the dithiocarbamate to the gold(I) center preserving the phosphine ligand, resulting in a linear coordination geometry. For all complexes, the NMR spectra showed characteristic signals of both the ligand and the precursors. In the ^{13}C NMR spectrum, complexation was mainly evidenced by the chemical shift of the signal corresponding to the −NCSS moiety within the coordination sphere. The remaining signals also shifted due to changes in electronic density caused by the introduction of gold into the structure. In the MDA-MB-231 cell line, the complexes exhibited IC_{50} values approximately two times lower than the free ligand, indicating that gold plays an important role in their antitumor activity. In summary, the desired products were successfully obtained and properly characterized by XRD and NMR and showed considerable cytotoxicity against cancer cell lines. Future perspectives include the investigation of the mechanisms of action through interactions with biomolecules.



a) Crystal structure of complex 1, b) Antiproliferative activity in MDA-MB-231 cancer cell line.

Agradecimentos/Acknowledgments

FAPEMIG, CNPq, CAPES, UFMG.

Structure–Activity Relationship in CO Photorelease by Ruthenium(II) Complexes with α-Diimine Ligands

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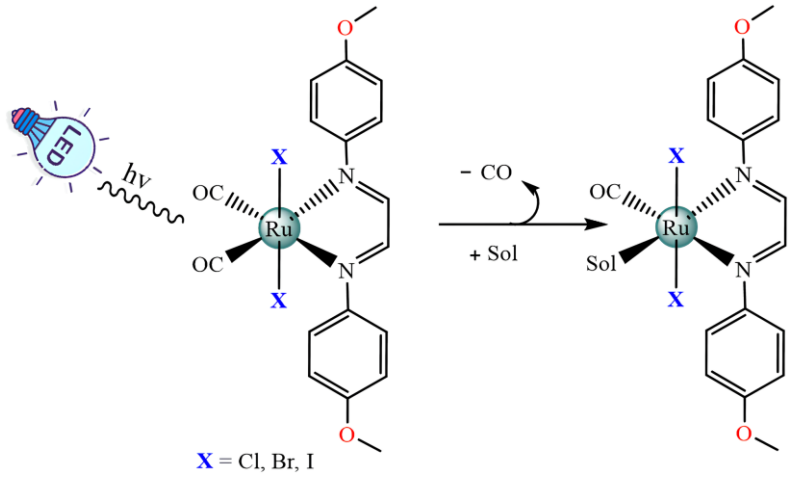
Palavras Chave:*ruthenium(II), halides, CO photorelease,ruthenium(II),,halides,,CO photorelease*

Highlights

All $RuX_2(CO)_2$OMe-DAB complexes were able to release CO upon blue and/or green LED irradiation. The variation of halides influences the rate of CO photorelease.

Resumo/Abstract

In recent years, studies involving metal ions have revolutionized the treatment of various diseases, especially following the discovery of the action of cisplatin. In this context, therapies based on carbon monoxide releasing molecules (CORMs) have emerged as versatile alternatives for photodynamic therapy. In this work, three new complexes with the general formula $RuX_2(CO)_2$OMe-DAB (X = Cl, Br, I) were synthesized for potential application as CO photoreleasing agents. These complexes were characterized using spectroscopic techniques and computational methods, and it was observed that the photoactive region lies within the visible spectrum, specifically in the blue and green wavelength ranges. Upon exposure to visible light irradiation, the synthesized complexes exhibited a decrease in the intensity of the two-characteristic*cis*-CO bands, while a lower-frequency band appeared during irradiation. This observation is consistent with the releaseof a carbonyl ligand from the coordination sphere and the formation of a new monocarbonyl species. The CO photorelease rates of the organometallic compounds were evaluated by FTIR band decomposition during light irradiation over time. From these data, it was possible to observe that the complex containing the bromide ligand displayed a faster release rate compared to the others. Although the variation of halides did not significantly alter the MLCT λmax, it was observed that they do influence the CO photorelease rate. The results obtained thus far demonstrate that the $RuX_2(CO)_2$OMe-DAB system stands out as a promising platform, particularly due to the ability of the complexes to release carbon monoxide at lower-energy wavelengths.



Proposed mechanism for the CO photorelease by $RuX_2(CO)_2$OMe-DAB complexes.

Agradecimentos/Acknowledgments

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Synthesis and catalytic evaluation of an LPMO-inspired copper catalyst

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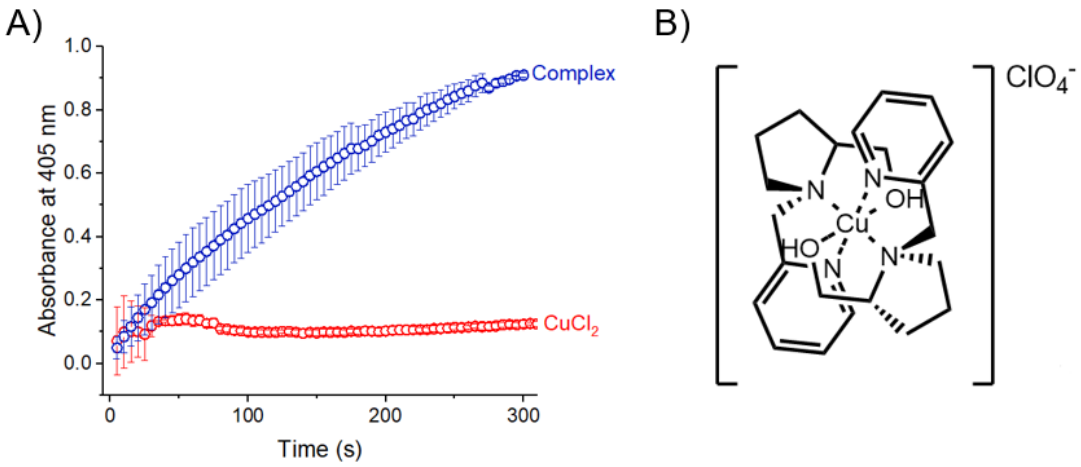
Palavras Chave:*Catalyst design,Bioinspired,Oxidative cleavage,Green chemistry,Model substrate*

Highlights

A copper catalyst was designed to mimic LPMO enzyme. It showed catalytic activity for oxidative glycosidic bond cleavage. This validates its design toward biomass conversion.

Resumo/Abstract

The search for sustainable energy sources and waste mitigation solutions highlights lignocellulosic biomass as a key renewable resource. In nature, enzymes like Lytic Polysaccharide Monooxygenase (LPMO) efficiently degrade biomass, but their large-scale use can be quite costly. To address this issue, we designed a synthetic copper catalyst mimicking the LPMO active site. We synthesized a new organic ligand with low steric hindrance which was coordinated with copper to create the novel bioinspired complex. Both the ligand and the complex were fully characterized. The ligand by 1D and 2D NMR, IR, UV-Vis and HRMS. The catalyst was analyzed by elemental analysis, HRMS, IR, UV-Vis, EPR and XPS, confirming its structure. The catalytic activity of the complex was first assessed qualitatively using p-nitrophenyl-β-D-glucopyranoside (PNp), a model substrate containing a β(1→4) glycosidic bond analogous to cellulose. Catalytic activity was confirmed by detecting the release of p-nitrophenolate ion, which has λ~405 nm. Later on, the catalyst was applied to real cellulose substrate in the form of filter paper. The successful breakdown was verified quantitatively by measuring the concentration of reducing sugars in the reaction medium using the 3,5-dinitrosalicylic acid (DNS) method. Positive results in both assays show the efficacy of the synthesized copper complex, validating its biomimetic design and establishing a promising basis for future studies with real lignocellulosic substrates.



Catalyst's activity profile in PNp cleavage, monitored by absorbance at 405nm (A) and structure (B).

Agradecimentos/Acknowledgments

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Synthesis and characterization of a new Ruthenium(II) complex with potential biological application

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Palavras Chave:*Ruthenium Complexes,Polypyridine Ligands,Synthesis,Characterization*

Highlights

Synthesis of*cis*-[Ru(bpy)(phen)(Amtz)$_2$](PF$_6$)$_2$complex, spectroscopic characterization by UV-Vis and infrared spectroscopy, electrochemical study of the RuIII/RuIIredox couple by cyclic voltammetry.

Resumo/Abstract

Ruthenium is a transition metal that has gained prominence in inorganic and medicinal chemistry due to its structural and biological properties. Ruthenium complexes containing polypyridyl and heterocyclic ligands have demonstrated promising antitumor, antibacterial, and antiviral activities, favoring the advancement of these compounds into clinical trial phases. This work proposes the synthesis and characterization of a new complex of the type*cis*-[Ru(bpy)(phen)(Amtz)$_2$](PF$_6$)$_2$, where Amtz = 2-amino-5-trifluoromethyl-1,3,4-thiadiazole, bpy = 2,2′-bipyridine, and phen = 1,10′-phenanthroline. Spectroscopic and electrochemical techniques were employed for characterization, as shown in Figure 1. UV–Vis and infrared absorption spectroscopic analyses provide indicative evidence of the formation and structural organization of the*cis*-[Ru(bpy)(phen)(Amtz)$_2$](PF$_6$)$_2$complex. The UV–Vis spectrum revealed bands typical of intraligand transitions at 229, 266, and 285 nm, and metal-to-ligand charge transfer transitions at 330, 444, and 469 nm; the observed shifts suggest the influence of the expected ligands, reinforcing coordination to the metal center. In the IR spectroscopy, vibrational bands attributed to specific functional groups (C=C, C=N, C–F, N–H) are consistent with the anticipated coordination modes, supporting the proposed structure of the complex. Additionally, the electrochemical study conducted by cyclic voltammetry using an Ag/AgCl reference electrode showed a half-wave potential ($E_1/_2$) of 617 mV, attributed to the RuIII/RuII redox couple. Thus, the obtained data indicate the structural integrity of the compound and support the formation of the desired complex. The research therefore seeks to contribute to the development of new, more selective and effective pharmacological alternatives.

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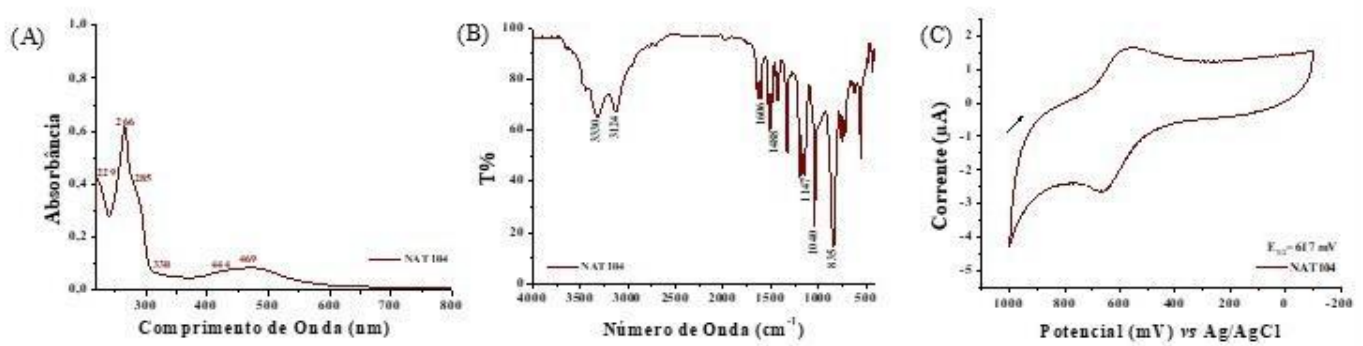


Figure 1. (A) UV–Vis in methanol; (B) IR (4000–400 cm^{-1}); (C) cyclic voltammogram.

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Synthesis and characterization of a novel cyclometalated ruthenium nitrosyl complex

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Palavras Chave:*ruthenium,cyclometalation,nitrosyl*

Highlights

The new cyclometalated compound [Ru(tpy-Cl)(η-bhq)NO]$(PF_6)_2$ is presented; the chloro substituent impacts the Ru-NO bond properties.

Resumo/Abstract

Nitric oxide (NO) is a crucial signaling molecule in various biological processes, which drives the development of NO-releasing molecules (NORMs) with therapeutic potential.[1] Cyclometalated (C^N) ligands possess σ-donor character in metal complexes, influencing chemical and biological properties such as increased lipophilicity and shifts in electronic levels when compared to their (N^N) analogs. Additionally, they allow for the modulation of the Ru-NO bond in nitrosyl complexes, depending on the substituents.[2] In this context, ligands such as benzo[h]quinoline directly influence the physicochemical and electronic properties of these metallodrugs.[3] This work is dedicated to the synthesis of the novel complex with the molecular formula [Ru(tpy-Cl)(η-bhq)NO]$(PF_6)_2$ (tpy-Cl = 4'-chloro-2,2':6',2'-terpyridine and bhq = benzo[h]quinoline) (**1**), and its characterization using techniques such as ^{1}H-RMN and COSY, FT-IR, UV-visible absorption spectroscopy and X-ray diffraction (XRD). The coordination of the NO ligand was confirmed by the typical stretching frequency NO at 1845 cm^{-1} (Figure 1a), and by ^{1}H-NMR (Figure 1b), which evidences the structure of the complex. When comparing the stretching frequencies of**1**with its previously synthesized analog [Ru(tpy)(η-bhq)NO]$(PF_6)_2$ (**2**),[4] a decrease of 12 cm^{-1} in the NO bond stretching is observed. This demonstrates that the chlorine substituent, which possesses electron-withdrawing character, decreases the π-acceptor capacity of the tpy, allowing for an increase in Ru-NO back-bonding and, consequently, the weakening of the NO bond. UV-Vis spectra (Figure 1c) showed intense absorption bands between 210 and 457 nm (log ε = 4.57-3.72). Future steps include XRD experiments to elucidate the octahedral geometry, lipophilicity via the partition coefficient (log P) and stability in aqueous media by the pK_a of the NO/NO^{2-} conversion.

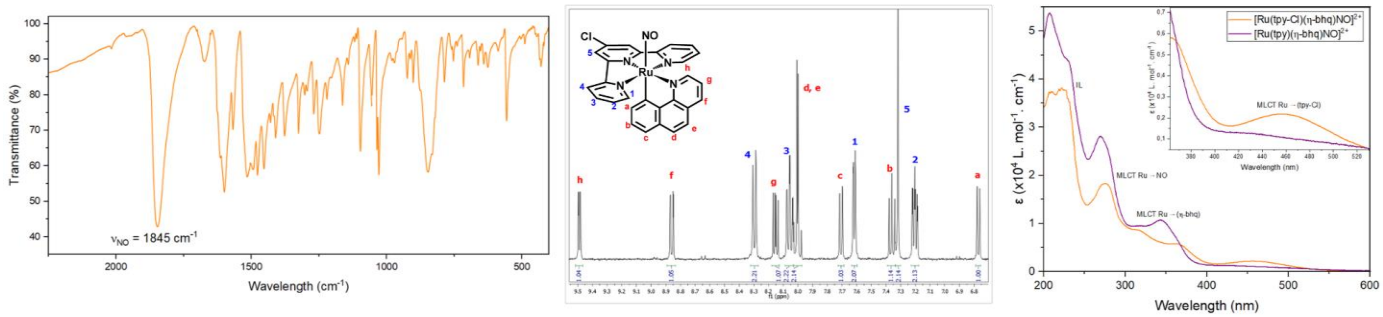


Figure 1. (a) Infrared spectrum (KBr); (b) 1H-NMR in CD3CN (1x10-2M); (c) UV-vis of 1 and 2 in MeCN.

Agradecimentos/Acknowledgments

This work was supported by the Brazilian agencies FAPESP and PUB - University of São Paulo.
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Synthesis and Characterization of a Ruthenium(II) Organometallic Complex Bearing a Furfural-Derived Schiff Base Ligand

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Palavras Chave:*Ruthenium(II) organometallic complex, coordination chemistry, furfural, Schiff base.*

Highlights

Synthesis of an iminic ligand derived from furfural

Synthesis of a complex containing a bidentate Schiff base

Resumo/Abstract

Schiff bases are versatile auxiliary ligands in coordination chemistry, particularly in catalytic applications. Herein, we report the synthesis and spectroscopic characterization of a Schiff base ligand and its use in the preparation of a Ru(II) organometallic complex with formula [RuCl(p-cymene)(1FUR)](PF_6). The ligand (1FUR) was obtained by condensation of equimolar amounts of furfural and*p*-toluidine in a C_3H_8O/H_2O mixture (75/5 mL) under stirring at room temperature for 24 h. After solvent removal, the product was isolated, washed with cold water, and dried under vacuum. FTIR spectroscopy confirmed ligand formation by the absence of the ν(C=O) band of furfural and the ν(N–H) band of*p*-toluidine, together with the appearance of the characteristic ν(C=N) band of the imine. UV-Vis spectroscopy revealed four absorption bands assigned to intraligand (IL) transitions. The Ru(II) complex was synthesized as a violet solid by refluxing toluene for 24 h using $[RuCl_2(p\text{-cymene})]_2$ (0.15 mmol), NH_4PF_6 (0.33 mmol), and 1FUR (0.33 mmol). The FTIR spectrum displayed bands consistent with the proposed coordination environment, including features of the Schiff base,*p*-cymene, and PF_6– counterion. A decrease in band intensities was observed upon complexation, along with a shift of the$\nu_{(C=N)}$ band from 1615 cm^{-1} to 1690 cm^{-1}, supporting Ru→N=C π back-donation. UV-Vis data (CH_2Cl_2 $6{,}64\times10^{-5}$ mol L^{-1}) showed three bands at 340 nm, 410 nm, and 500 nm, assigned to IL and MLCT transitions. Conductivity measurements in CH_2Cl_2 at 25 °C (1×10^{-3} mol L^{-1}, Λm: 20,33 ohm^{-1} cm^2 mol^{-1}) indicate 1:1 electrolytic behavior, consistent with the proposed mononuclear cationic structure. These results support the coordination environment of the target complex.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG, and UFU

Synthesis and characterization of copper-based electrocatalysts for water oxidation

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Palavras Chave:*: oxidação de água, evolução de oxigênio, complexos de cobre.,Water oxidation,Oxygen Evolution Reaction,Copper complexes*

Highlights

Copper complexes as low-cost alternatives to Ru catalysts for water oxidation. Synthesis and characterization of copper complexes.

Resumo/Abstract

The progressive increase in greenhouse gas emissions associated with the use of fossil fuels has intensified the search for more sustainable energy sources. Among these, water electrolysis for hydrogen production stands out as a clean and promising alternative. In this context, the oxygen evolution reaction (OER) represents the main rate-limiting step of the process, due to its slow kinetics and the high potentials required for O–O bond formation. Although ruthenium-based complexes exhibit high catalytic efficiency for water oxidation, their high cost and low abundance motivate the development of catalysts based on more abundant metals, such as copper. Thus, this work aims at the synthesis, characterization of a copper coordination complexe containing modified pyridinic ligand and Schiff bases, targeting their application in the electrocatalytic oxidation of water. Mononuclear complexes of the [Cu(N–N–N–N)] types will be investigated, with emphasis on the influence of the electronic and structural properties of the coordination sphere on catalytic efficiency and the O–O bond formation mechanism. Preliminary results demonstrate the successful synthesis of the Schiff base bendipyr ((1E,1′E)-N,N′-(1,2-phenylene)bis(1-(1H-pyrrol-2-yl)methanimine)) and its corresponding copper complex [Cu(bendipyr)], confirmed by NMR spectroscopy and high-resolution mass spectrometry. Subsequent stages include electrochemical characterization, quantification of oxygen generation, advanced spectroscopic studies, and theoretical simulations of reaction intermediates, aiming to elucidate the general mechanism of water oxidation by copper complexes and to provide a foundation for the rational design of new, more efficient and energetically accessible catalysts.

Agradecimentos/Acknowledgments

CAPES, CNPQ, FAPESP e IQ-UNICAMP

Synthesis and Characterization of Core@Shell Systems Based on Metallic NPs@MOFs and Rare-Earth Doping

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Palavras Chave:*UiO-66-NH2,gold nanoparticles,hybrid system,magnetite*

Highlights

Synthesis and characterization of hybrid core@shell systems, combining MOFs and metallic nanoparticles into a multifunctional platform with potential theranostic applications.

Resumo/Abstract

Metal–organic frameworks (MOFs) and metallic nanoparticles have been widely investigated due to their complementary properties, including high porosity, large surface area, and optical, magnetic, and photothermal functionalities. Their integration into core@shell architectures enables the development of multifunctional systems with expanded applications. Among these, controlled drug delivery platforms have attracted attention for oncological therapies.[1] such as breast cancer. In this work, metallic nanoparticles and MOF-based hybrid systems were synthesized. Gold nanoparticles (AuNPs) were prepared by chemical reduction using sodium citrate as reducing and stabilizing agent. Iron oxide nanoparticles were synthesized via coprecipitation of Fe(II) and Fe(III) ions with NH_4OH, targeting magnetic applications. The MOF UiO-66-NH_2 was obtained by a solvothermal method using $ZrCl_4$ and 2-aminoterephthalic acid (BDC-NH_2). Using pre-formed nanoparticles as seeds, UiO-66-NH_2 growth was promoted on their surfaces, forming AuNP@UiO-66-NH_2 and Fe_3O_4@UiO-66-NH_2 core@shell systems. The formation of UiO-66-NH_2 was confirmed by X-ray diffraction, showing peaks at approximately 7°, 8°, and 12°, assigned to the (111), (200), and (220) planes. Magnetite formation was verified by peaks at 30°, 35°, and 62°, corresponding to the (220), (311), and (440) planes. AuNPs exhibited a UV–Vis band centered at 520 nm, indicating an average particle diameter of 20–25 nm. These core@shell architectures combine the structural stability of UiO-66 with the photothermal and magnetic core@shell architecture combines the structural stability of UiO-66 with the photothermal and magnetic properties of AuNPs and Fe_3O_4, yielding promising hybrid systems. Future Eu^{3+} doping is expected to introduce luminescent functionality and further enhance theranostic performance.[2]

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Agradecimentos/Acknowledgments

FAPESP (2025/24167-9), CNPq (20239/2025-8, 309448/2021–2, 305313/2024-0 and 308868/2022-6), and BSTR.

Synthesis and Characterization of Gold Nanoparticles Incorporated into Palladium(II)–Thiosemicarbazone Complexes: DNA Interaction Studies

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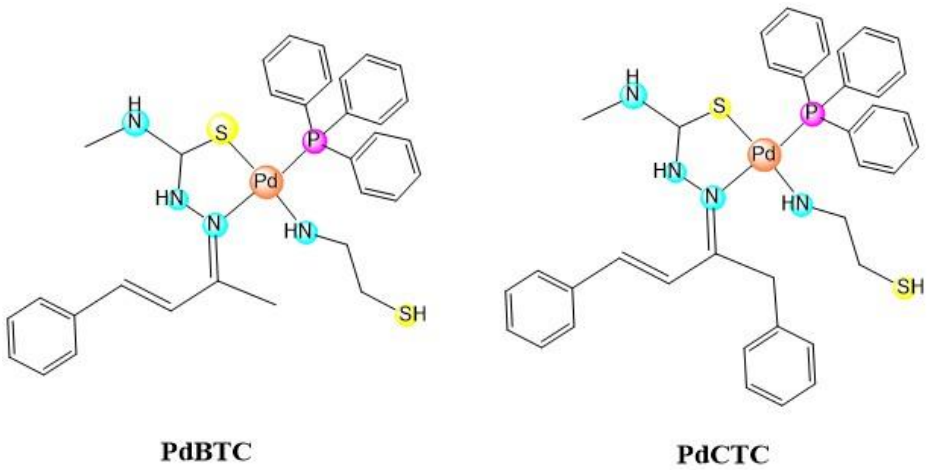
Palavras Chave:*Metal complexes,Palladium,Gold nanoparticles,Thiossemicarbazones,Cancer*

Highlights

Synthesis and characterization of Pd(II) complexes incorporating AuNPs, explored as nanocarriers for palladium-based anticancer agents. Evaluation of DNA interaction as a potential biological target.

Resumo/Abstract

Cancer is a group of more than 100 diseases characterized by the disordered growth of cells that have undergone nuclear changes and can no longer perform their original function. There is an increasing need to develop new drugs to overcome the issues observed in platinum complexes, and palladium is proving to be a promising alternative due to its physicochemical properties that are similar to platinum's. In this work, two palladium(II) complexes containing a cysteamine spacer (PdBTC and PdCTC) were synthesized and fully characterized using spectroscopic techniques. UV–Vis spectroscopy revealed characteristic absorption bands in the 380–400 nm and 490 nm regions, consistent with ligand coordination to the palladium center. Infrared spectroscopy further supported metal–ligand coordination. The 1H nuclear magnetic resonance (NMR) experiment revealed the coordination of the ligands to the palladium metal center and of the proposed spacer to the metal through chemical shifts and peaks. A stability test using 31P NMR indicated that the proposed complexes are stable in dimethyl sulfoxide (DMSO), a solvent accepted for future biological tests. Finally, a test will be performed using the spectrophotometric titration technique to study possible interactions with DNA. This technique seeks to extract quantitative information about the interaction between the complexes and DNA. It will verify whether the interaction occurs covalently, electrostatically, or by intercalation. This will be done by evaluating the intrinsic binding constant (Kb). The test will also determine if replacing the Cl ligand with the cysteamine spacer influences the interaction of the complex with DNA.



Estrutura dos complexos sintetizados e caracterizados (PdBTC e PdCTC)

Agradecimentos/Acknowledgments

CNPq (305259/2025-3), FAPESP

Synthesis and characterization of ruthenium-cymene complexes containing β-diketonate and phosphine ligands

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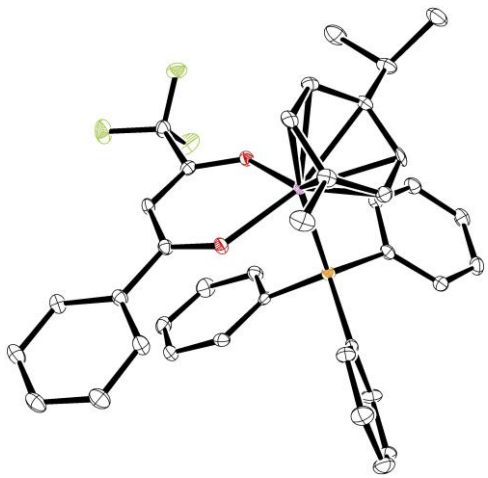
Palavras Chave:*Ruthenium,β-diketonates,Phosphines,Organometallic synthesis,Spectroscopic and structural characterization*

Highlights

Novel Ru(II) organometallic complexes synthesis.
Bidentate β-diketonate and phosphine coordination.
Characterization by NMR and X-ray diffraction.
Potential agents for biological evaluation.

Resumo/Abstract

Ruthenium(II) arene complexes have gained prominence in coordination chemistry due to their structural versatility. This work describes the synthesis and structural characterization of a series of novel organometallic complexes with the general formula [Ru(η⁶-*p*-cymene)(BTA)PR_3]PF_6 (BTA = 4,4,4-trifluoro-1-phenyl-1,3-butanedione, and R = Ph –**1**,*p*-F-Ph –**2**,*p*-tol –**3**and*p*-anisol –**4**). These complexes were obtained by the reaction of [Ru(η⁶-*p*-cymene)(BTA)Cl] in MeOH and the corresponding triarylphosphine ligands in the presence of $AgPF_6$. All complexes were characterized by multinuclear NMR (^{1}H, ^{13}C and ^{31}P{^{1}H}), vibrational and electronic spectroscopy, molar conductivity, and single-crystal X-ray diffraction (SC-XRD). The ^{31}P{^{1}H} NMR spectra exhibited one singlet in the region of 29.8 and 31.9 ppm, confirming phosphine coordination. All coordinated triarylphosphine ligands are deshielded compared to the free ligands with coordination shifts (Δδ) up to 41.9 ppm. The chemical shifts were sensitive to the electronic nature of the PR_3 substituents, where electron-donating groups (OMe and Me) promoted greater shielding of the phosphorus nuclei compared to the electron-withdrawing fluorine substituent. The detection of a characteristic septet at δ -144.2 ppm confirmed the presence of the PF_6^- counter-ion in the outer sphere. Structural elucidation of four complexes in the series by XRD revealed piano-stool geometries (monoclinic and triclinic systems), with the β-diketonate ligand chelated to the metal center. These results establish the structural identity of the new complexes for future biological activity evaluations.



[Ru(η6-p-cymene)(BTA)(PPh3)]PF6 (1) by XRD (ellipsoids at 30%; PF6- and H are omitted).

Agradecimentos/Acknowledgments

This work was supported by PPGQ-UFPR, with technical support from DRXm-UFPR for crystallographic data collection, and a research fellowship provided by CNPq.

Synthesis and Characterization of Silver Nanowires: Effect of NaCl, NaBr, and Fe(NO3)3 on Structural Homogeneity

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Palavras Chave:*Nanofios de prata,,Síntese e Caracterização,,Método Poliol,,Silver Nanowires,,Synthesis and Characterization,,Polyol Method,,Nanomaterials,*

Highlights

AgNW synthesis via polyol method with precise NaCl/NaBr and $Fe(NO_3)_3$ morphology control. Comparative study of NaCl and NaBr as salt mediators in silver nanowire synthesis.

Resumo/Abstract

Silver nanowires (AgNWs) are one-dimensional nanomaterials of significant relevance due to their high electrical and thermal conductivity, combined with unique optical properties. Their morphology enables the creation of transparent percolative networks, making them ideal for applications in flexible electronics, solar cells, and high-performance sensors. Morphological control is crucial to ensure efficiency in these applications, therefore, this work aimed to verify the influence of sodium salts (NaCl or NaBr) on the dimensions of the wires and the effectiveness of $Fe(NO_3)_3$ as a directing agent for the interaction between the polymer and the metallic surface. The synthesis was performed using the polyol method, with ethylene glycol (EG) as the solvent and reducing agent, polyvinylpyrrolidone (PVP) as the stabilizer, and $AgNO_3$ as the silver ion source. The PVP solution is heated for 1 hour at 170°C, followed by the addition of the NaCl or NaBr solution, and then the $Fe(NO_3)_3$ solution is added or omitted. $AgNO_3$ is slowly added via a syringe pump over 1 hour; upon completion of the injection, the reaction proceeds under heating for 35 minutes. The purification process included three washing cycles each with acetone and ethanol, aided by centrifugation and ultrasonication. TG/DSC analysis showed a total mass loss of less than 1.5% up to 600°C in the samples, evidencing the efficiency of the purification processes in removing solvents and excess organic reagents. FTIR analyses confirm the presence of characteristic PVP bands at 1650 cm^{-1}, corresponding to the C=O stretching of a cyclic amide, indicating the coordination of the polymer to the metallic silver surface. SEM and TEM analyses are expected to confirm greater morphological homogeneity in the samples with iron, in addition to distinguishing variations in diameter and PVP layer thickness depending on the halide used. Surface area and porosity will be quantified via ASAP.

Agradecimentos/Acknowledgments

CNPq, CAPES, Petrobras

Synthesis and Characterization of Single Crystals Containing Rare-Earth Ions Derived from Electronic Waste for Magneto-Optical Applications.

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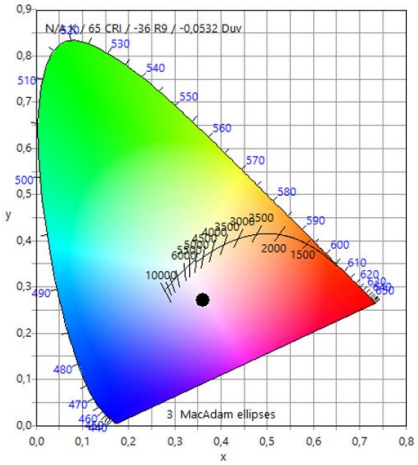
Palavras Chave:*terras-raras,resíduos-eletrônicos,garnets,propriedades magneto-opticas*

Highlights

Sustainable synthesis of rare-earth garnet single crystals from recycled fluorescent lamp waste for luminescent and magneto-optical applications.

Resumo/Abstract

The growing global demand for rare earth elements (REEs), along with the environmental impacts associated with their extraction, has stimulated the search for alternative and sustainable routes, such as urban mining. In this work, gallium-based garnet single crystals (RE:GGs) containing rare earth ions recovered from fluorescent lamp waste (e-waste) were synthesized and characterized for magneto-optical and luminescent applications. The crystals were obtained from a glass-ceramic matrix based on $PbO–GeO_2–Bi_2O_3–Ga_2O_3$ with the addition of 3, 5, and 7% of electronic waste, employing controlled heat treatments to promote nucleation and crystal growth. The glass composition was melted at 1450 °C for 1 hour and cooled to 1100 °C for the nucleation and crystal growth step. The extraction of single crystals was performed by chemically etching the glassy phase with a concentrated HCl solution. The chemical composition of the e-waste was determined by inductively coupled plasma mass spectrometry (ICP-MS), revealing the presence of 37 elements, including Y, Tb, and Eu. For the crystals, Scanning electron microscopy analyses indicated crystals with sizes ranging from 20 to 40 µm, while elemental mapping by energy-dispersive X-ray spectroscopy (EDS) confirmed the incorporation of rare earth ions, Eu and Tb. Photoluminescence measurements evidenced characteristic transitions of Eu^{3+} and Tb^{3+}, specifically the Eu^{3+} $^5D_0 \rightarrow {}^7F_1$, $^5D_0 \rightarrow {}^7F_2$ and $^5D_0 \rightarrow {}^7F_4$ transitions, as well as the Tb^{3+} $^5D_4 \rightarrow {}^7F_6$ and $^5D_4 \rightarrow {}^7F_5$ transitions, enabling the construction of the CIE 1931 chromaticity diagram and indicating emission in the warm white region. These results demonstrate the high potential of reusing e-waste to obtain high-performance luminescent materials, contributing to sustainable strategies for the development of advanced photonic devices.



As coordenadas de cromaticidade CIE 1931 foi obtido a partir do espectro de emissão.

Agradecimentos/Acknowledgments

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Synthesis and characterization of Tb^{3+}-doped no-core fiber for optical and magneto-optical applications

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Palavras Chave:*Optical fibers,Borogermanate glasses,Terbium,Magneto-optical,Optical sensors*

Highlights

Tb^{3+}-doped borogermanate glasses and glass perform synthesized by melt-quenching process; Fabrication of high-loss no-core fiber containing high concentration of Tb^{3+} ions;

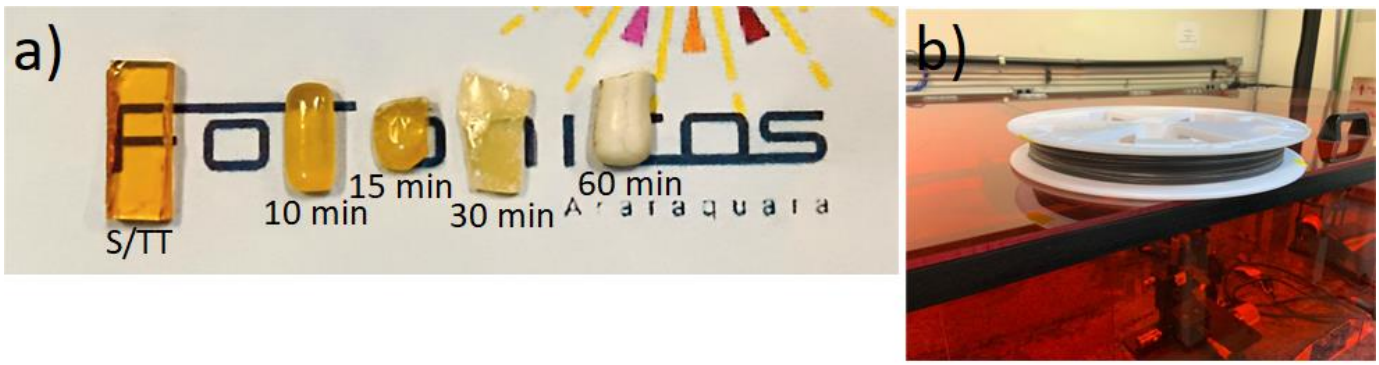
Resumo/Abstract

Distributed optical fiber sensors (DOFS) enable continuous and spatially resolved monitoring of physical parameters by exploiting intrinsic light scattering phenomena along optical fibers, in which the fiber itself acts as the sensing element [1]. Rayleigh scattering originates from microscopic refractive index fluctuations in the glass structure, and microcrystals act as additional scattering centers [1]. This work reports the fabrication of a single no-core optical fiber with high optical signal attenuation and the synthesis and characterization of Tb^{3+}-doped borogermanate glass-ceramics. Analysis of the glass-ceramics made it possible to identify the crystals within the fiber structure. The no-core fiber was fabricated from a BGB-10 mol% Tb_4O_7 glass preform using the melt-quenching technique and fiber drawing. During the fiber drawing process, a crystallization process was identified within the fiber. Glass-ceramics were synthesized at 860 °C for 10, 15, 30, and 60 minutes to induce controlled crystallization. The glass-ceramics were characterized by X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS), differential scanning calorimetry (DSC), and photoluminescence spectroscopy (PL). XRD revealed $BaAl_2O_4$ and Tb_2O_3 phases in the glass-ceramics, which are the same crystalline phases found within the fiber. SEM/EDS showed 5–10 µm crystals containing Ba, Al, and Tb. DSC curves indicated a reduction of ΔT from 242 to 214 °C after the crystallization process. PL spectra showed Tb^{3+} electronic transitions with Stark splitting at 545 nm, confirming ion incorporation into ordered crystalline environments [2]. The successful manufacture of a no-core fiber confirms the potential of this system for optical applications requiring high signal attenuation and distributed sensing.

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2. Franco, D.F.*et al.*Materials, 18, 4736 (2025).



(a) BGB-10Tb glass-ceramics heat-treated at 860 °C and (b) BGB-10Tb optical fiber

Agradecimentos/Acknowledgments

The authors thank CNPq/PROPe/PIBITI and FAPESP (process 2023/04832-2) for financial support, and the LaViE and LAMF research groups and IQAr-Unesp for infrastructure and technical assistance.

Synthesis and Characterization of Tetra-RuthenatedMetalloporphyrins Bearing Bisphosphine Ligands:Phototoxicity and DNA Interaction Studies

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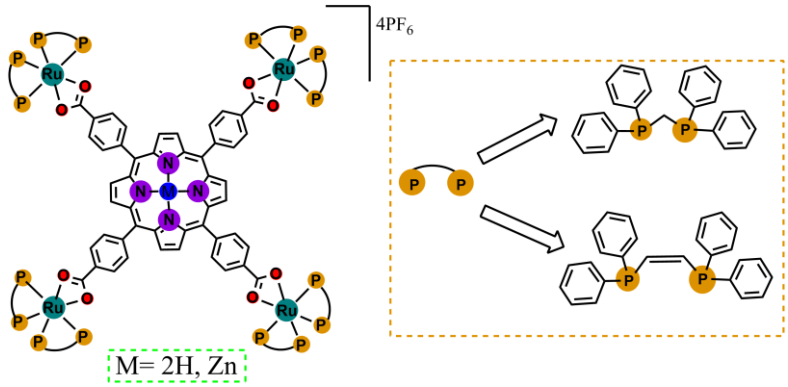
Palavras Chave:*Cancer,Coordination Chemisty,Porphyrin,Photodynamic Therapy*

Highlights

- Synthesis and full characterization of novel tetra-ruthenated metalloporphyrins.
- Ruthenium(II) bisphosphine fragments as peripheral functionalization for PDT.
- Evaluation of DNA interaction.

Resumo/Abstract

Cancer is a group of diseases characterized by the uncontrolled proliferation of abnormal cells, which can form masses of cells (tumors) or invade adjacent tissues (metastasis), the latter of which is one of the leading causes of death. Intravenous chemotherapy and photodynamic therapy (PDT) are two of the most notable available therapies. PDT involves the irradiation of a photosensitizer (PS) in the visible region, generating reactive oxygen species (ROS) that can induce cell apoptosis. This work describes the synthesis and characterization of new porphyrin-based (PS) compounds. These compounds are formed by combining porphyrins, which have intrinsic photophysical properties, with ruthenium(II) ions coordinated to bisphosphine ligands at their peripheries. Additionally, we synthesized analogues with zinc(II) ions at the center of the macrocyclic ring. The goal was to expand the mechanisms of action and enhance the intrinsic photophysical properties of the compounds. Spectroscopic techniques, such as NMR experiments (^{1}H and $^{31}P\{^{1}H\}$), were used to elucidate the structure of the synthesized compounds. These experiments verified the coordination by identifying the signals present in the spectra and the difference in chemical shift after the coordination of the metal ions. UV-Vis spectroscopy identified the characteristic bands of this class of compounds: the Soret band between 415 and 430 nm and the four Q bands between 500 and 680 nm. Titration experiments with calf thymus DNA (ct-DNA) were performed to investigate the interaction with DNA, indicating a weak binding affinity based on the calculated binding constants (Kb). However, cytotoxicity assays with ovarian cancer cell lines revealed significant anticancer activity only under light irradiation at 416 nm, underscoring the photodynamic nature of these compounds. Complementary studies, including DNA photocleavage assays, are ongoing and aim to further elucidate the mechanisms of action of these light-activated.



General structure of synthesized compounds and bisphosphines used.

Agradecimentos/Acknowledgments

CNPq (305259/2025-3), FAPESP

Synthesis and crystal structures of new lanthanide(III) coordination compounds containing 3-thiophenecarboxylate and 2,2'-bipyridine as ligands

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Palavras Chave:*lanthanides, X-ray diffraction, coordination chemistry*

Highlights

New binuclear lanthanide complexes with 3-thiophenecarboxylate as a ligand were synthesized via a one-pot method in order to investigate their spectroscopic and magnetic properties.

Resumo/Abstract

Multifunctional compounds have been widely studied in recent decades due to their potential applications in different fields and the ability of a single material to perform multiple roles within the same system.[1] In this context, lanthanide complexes are particularly attractive, due to their possible interesting magnetic and optical properties.[2] Although the emission of lanthanide ions is usually weak, it can be intensified when coordinated to antenna ligands, which transfer energy to the lanthanide excited levels. In this work, a new series of lanthanide-based complexes with 3-tiophenecarboxylate (3tca) and 2,2'-bipyridine (bpy) as ligands was synthesized. The compounds were obtained by a one-pot method in an ethanol/water (2:1) mixture. Bpy, 3tca, and the corresponding lanthanide nitrate (Sm^{3+} (**1**), Eu^{3+} (**2**), Gd^{3+} (**3**), Tb^{3+} (**4**), Dy^{3+} (**5**), and Er^{3+} (**6**)) were mixed in a 1:3:1 molar ratio and refluxed. After 21 days of slow evaporation of the mother liquor, single crystals suitable for X-ray diffraction analysis were isolated. The crystal structure of**1**has already been determined; the other measures and refinements are ongoing. Compound**1**crystalized in a P triclinic space group and consists in a binuclear structure of formula $[Sm_2(3tca)_4(bpy)_2(NO_3)_2]$, as represented in**Fig. 1**. Thus, the final complex shows a 1:2:1 stoichiometry. The lanthanide ions are coordinated by both oxygen atoms of one 3tca ligand, and one oxygen atom from each other ligand. In addition, two bpy nitrogen atoms and nitrate oxygen atoms fill the coordination spheres. No coordinated water molecules were observed. Magnetic and luminescent properties are under investigation.

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[2]Areas, E. et al.,*J. Braz.Chem. Soc.***, 2024**, 35, e-20230160.

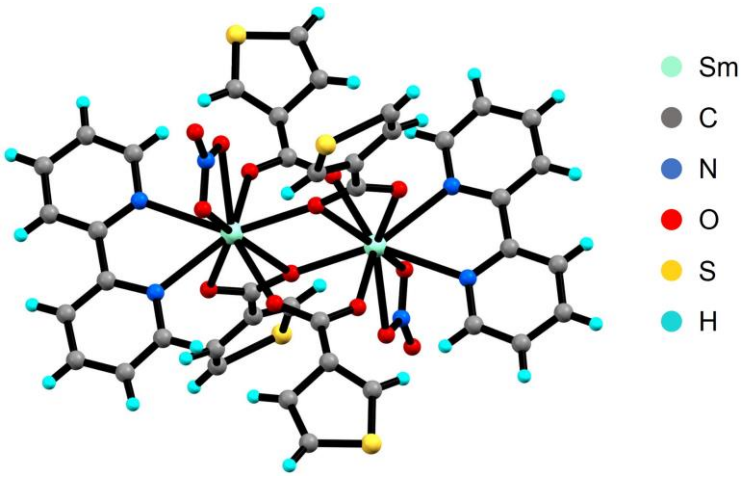


Fig. 1. Crystal structure of compound 1.

Agradecimentos/Acknowledgments

CAPES, FAPERJ, CNPq, LDRX-UFF, and LAME-UFF.

Synthesis and spectroscopic properties of lanthanide(III) complexes with 2-bromo-3-thiophenecarboxylate and 1,10-phenantroline as ligands

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Palavras Chave:*lanthanides,X-ray diffraction,coordination chemistry*

Highlights

Lanthanide compounds containing the ligands 2-bromo-3-thiophenecarboxylate and 1,10-phenanthroline were synthesized under reflux. Their structures were determined by single-crystal X-ray diffraction.

Resumo/Abstract

Ligantes orgânicos combinados com metais de transição podem gerar materiais com características multifuncionais, sendo elas ópticas, magnéticas, entre outras.[1] Neste trabalho, foi empregado o 2-bromo-3-tiofenocarboxilato (3tcaBr) como ligante em uma série de complexos contendo íons lantanídeo(III), tendo a 1,10-fenantrolina (phen) como ligante auxiliar. Foram obtidos seis complexos de lantanídeos com o ligante 3tcaBr, de fórmula geral $[Ln_2(3tcaBr)_4(phen)_2(NO_3)_2]$ (onde Ln= Sm^{3+} (**1**), Eu^{3+} (**2**), Gd^{3+} (**3**), Tb^{3+} (**4**), Dy^{3+} (**5**) Er^{3+} (**6**)) a partir da reação entre 3tcaBr, phen e o nitrato do respectivo lantanídeo em uma razão estequiométrica 3:1:1. A mistura permaneceu em refluxo em uma solução 9:1 EtOH/dmf. Os compostos**1**e**4**geraram monocristais após cerca de 15 dias de evaporação lenta das soluções reacionais, sendo caracterizados por difração de raios X e espectroscopia de absorção na região do infravermelho; os demais foram obtidos na forma de policristais e caracterizados por difração de raios X por policristais. A partir dos dados obtidos por difração de raios X, foi possível determinar que os compostos**1**e**4**cristalizaram no sistema triclínico, com grupo espacial P . A análise dos difratogramas indicou que os demais compostos são isomórficos. Os compostos são binucleares, e cada íon lantanídeo é coordenado por um átomo de oxigênio de cada ligante 3tcaBr, pelos dois átomos de oxigênio de um coligante nitrato e pelos dois de nitrogênio de um coligante phen (**Fig.1**). A análise dos espectros de infravermelho evidenciou a presença de bandas características atribuídas ao estiramento assimétrico das ligações no grupo carboxilato, observadas em aproximadamente 1630 cm^{-1}.[2] O estudo dos compostos utilizando a espectroscopia de emissão e cálculos teóricos está em andamento.

[1] AREAS, E. et al., J. Braz. Chem. Soc.,**2024**, 35, e-20230160.

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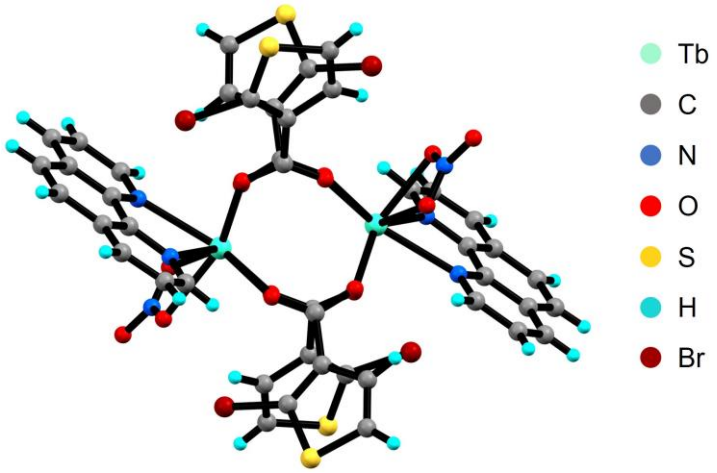


Fig 1. Estrutura do composto 4.

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES, LDRX-UFF, and LAME-UFF.

Synthesis, characterization and anticancer activity of Nitro-Vanillin-Derived thiadiazoles and oxadiazoles

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Palavras Chave:*Thiosemicarbazone, Thiadiazole, oxadiazole, Nitric Oxide, anticâncer*

Highlights

Synthesis and characterization of thiadiazoles and oxadiazoles by reaction of thiosemicabazones and semicarbazone with NO/O2; investigation of the cellular viability of these compounds in tumor cells

Resumo/Abstract

Cancer is a disease that accounts for over 12% of deaths worldwide. In advanced cases of the disease, radiotherapy using drugs such as cisplatin and 5-Fluorouracil (5-FU) is recommended. This treatment is aggressive for the patient and has several side effects. Therefore, the search for new therapeutic strategies is essential. In this work, we present the synthesis and characterization of nitro-vanillin derivatives thiadiazoles and oxadiazoles to develop potential antitumor agents. The insertion of a nitro (NO_2) group into these compounds aims to enhance the pharmacological effects of these compounds, especially under hypoxic conditions. The synthesis of nitro compounds was carried out by forming nitrovanillin using the novel NO/O_2 bubbling method in solution. Thiosemicarbazones and semicarbazones derived from vanillin nitro-vanillin were synthesized in acetic acid medium (70 °C). The syntheses of cyclocompounds were obtained by reaction between TSC (or SC) and NO/O2. The IR spectra display all characteristic bands present in the TDZ and OXD structures. The presence of two signals at (1532 cm-1) and (1355 cm-1) corresponds to the nitro group of these compounds. The 1H NMR spectra show all peaks along with the disappearance of a doublet, suggesting the entry of the NO2 group into the aromatic ring. Mass spectrometry and elemental analysis confirm the entry of the NO2 group and loss of two H, matching precisely with molecular masses and percentages of the TDZ and OXD. The cytotoxicity effects of the compounds were tested in assays using the human tumor cell (A549) with cell viability of 50-70% and normal cells (MRC5) with 80%.

Agradecimentos/Acknowledgments

We thank FAPESP and CNPq for funding this research.

Synthesis, characterization and antiproliferative activities over melanoma (SK-MEL-28) and squamous carcinoma (SCC-25) cells of a novel Zn(II) complex

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Palavras Chave:*Zinc(II),6-Trifluoromethyluracil,Melanoma,Squamous cell carcinoma,Antitumor activity*

Highlights

1. A novel zinc complex with 6-trifluoromethyluracil was synthesized
2. Coordination of the ligand to zinc occurs by nitrogen and oxygen atoms
3. The complex was active over SK-MEL-28 and SCC-25 cells

Resumo/Abstract

Skin cancer is the most common malignant neoplasm, which comprises about 30% of all cancer cases[1]. Nucleobase analogs as, for example 5-fluorouracil (5-FU), have been used in some types of cancer. One strategy in the development of new antitumor agents comprises the coordination of bioactive metals with ligands that already possess medicinal properties such as nucleobase analogs. Considering this approach, zinc(II) remains an attractive yet unexplored metal with therapeutic potential. In this context, the present work reports the synthesis, characterization and in vitro antiproliferative study of a novel zinc(II) complex containing the nucleobase analogue 6-trifluoromethyluracil (6-TFMU).

The Zn(II) complex was prepared via deprotonation of 6-TFMU (1.0 mmol) in alkaline aqueous medium, followed by addition of Zn(II)-bipyridine prepared early (0.50 mmol). Crystals were obtained from the solution after slow evaporation at room temperature for one week. Elemental analysis confirmed the composition as $C_{20}H_{14}ZnF_6N_6O_5$. Anal. Calcd. for $C_{20}H_{14}ZnF_6N_6O_5$: C 40.19; H 2.36; N 14.06. Found(%): C 40.23; H 1.49; N 13.93%. Single crystal X-ray diffraction, IR and RMN data confirmed coordination of 6-TFMU to zinc by one carbonyl oxygen and one amine nitrogen atom.

Antiproliferative activity was primarily evaluated against SK-MEL-28, SCC-25, and immortalized keratinocyte (HaCaT) cell lines using a colorimetric assay, with cisplatin and 6-TFMU serving as controls. Cell growth inhibition was determined by absorbance at 540 nm, and IC_{50} values were calculated by sigmoidal regression. The complex showed moderate antiproliferative activity over SK-MEL-28 and SCC-25 cells, with IC_{50} values ranging from 20 to 200 µM, while cisplatin showed IC_{50} values of 13.5 and 17.7 µM, for the same cells, respectively. Further studies are envisaged to expand biological evaluation of the zinc(II) complex over tumoral cells including biophysical assays.

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Agradecimentos/Acknowledgments

Acknowledgments: The authors acknowledge the Brazilian Agencies FAPESP (2025/01640-0 and 2021/10265-8 Cancer Theranostic Innovation Center CEPID CancerThera), CNPq (304661/2024-4) and CAPES.

Synthesis, Characterization and Pre-Catalytic Evaluation of a Vanadyl Diimine–Acetylacetonate Complex

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Palavras Chave:*Palavras Chaves:, íoin vanadilo, ácido fórmico, produção de gás hidrogênio, catálise homogênea.,Vanadyl ion,formic acid,hydrogen gas production,homogeneous catalysis*

Highlights

A new vanadyl complex was synthesized and fully characterized; IR, UV–Vis and conductivity support a 1:1 electrolytic structure; promising pre-catalyst for formic acid dehydrogenation.

Resumo/Abstract

Metal complexes containing the vanadyl ion have attracted considerable interest in coordination chemistry due to their structural properties and potential applications in homogeneous catalysis. The catalytic decomposition of formic acid (FA) to produce H_2 and CO_2 has been known for approximately 75 years and has been widely investigated in homogeneous catalytic systems. In this work, the synthesis and characterization of the complex [VO(acac)(2,4,6-trime)]PF_6 are reported, where 2,4,6-trime corresponds to the ligand N¹,N²-bis(2,4,6-trimethylphenyl)ethane-1,2-diimine and $acac^-$ to the acetylacetonate anion. The complex was synthesized by reacting one equivalent of the precursor [VO(acac)$_2$] (50 mg, 0.1885 mmol) with 1.2 equivalents of the diimine ligand (66 mg, 0.2257 mmol) in a mixture of ethanol (20 mL) and dichloromethane (10 mL), under reflux for 24 h. Subsequently, an excess of NH_4PF_6 was added, and the mixture was refluxed for an additional 1 h. The product was isolated after solvent evaporation, washing with cold water and diethyl ether, and drying under vacuum. The complex was characterized by spectroscopic and physicochemical techniques. The infrared spectrum showed bands at 555 cm^{-1}, attributed to the ν(V=O) stretching vibration, at 1523 cm^{-1} corresponding to the ν(C=O) stretch of the $acac^-$ ligand, at 831 cm^{-1} assigned to the ν(P–F) stretch of th e PF_6^- counterion, and at 1568 cm^{-1} characteristic of the ν(C=N) stretch of the diimine ligand. Molar conductivity measurements in dichloromethane and methanol indicated 1:1 electrolytic behavior. The UV–Vis spectra of [VO(acac)$_2$] and [VO(acac)(2,4,6-trime)]PF_6 exhibited a single band at 324 nm, with molar absorptivities of 50.84 and 59.04 $L \cdot mol^{-1} \cdot cm^{-1}$, respectively, consistent with d–d transitions. Overall, the results support the proposed structure, and preliminary tests indicate that the complex is a promising pre-catalyst for formic acid conversion to hydrogen.

Agradecimentos/Acknowledgments

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Synthesis, characterization, and reactivity of a new nitrosylsulfite complex trans-[Ru(NH3)4(pz)(N(O)SO3)](PF6)

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Palavras Chave:*Ruthenium,Nitrosylsulfite,Pyrazine*

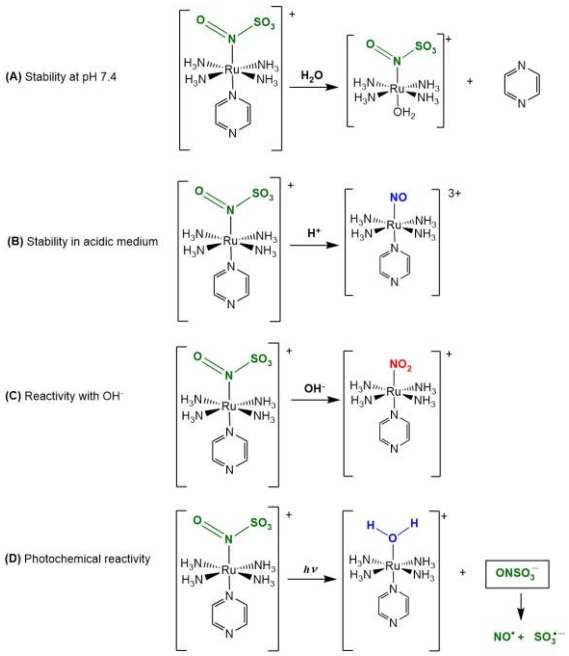
Highlights

A new ruthenium(II) tetraamine nitrosylsulfite complex was synthesized and characterized.

Pyrazine coordination trans to $N(O)SO_3^-$ strongly influences ligand stability and reactivity.

Resumo/Abstract

This work aims to investigate the reactivity of the nitrosylsulfite ligand, $N(O)SO_3^-$, coordinated to ruthenium complexes of the general formula*trans*-$[Ru(NH_3)_4(L)(N(O)SO_3)]^+$, with emphasis on their stability, aqueous reactivity, and chemical and photochemical properties. Although still scarcely explored, this class of complexes is of interest due to its ability of releasing both nitric oxide (NO•) and sulfite radical anion ($SO_3^{\bullet-}$) upon photolysis, with potential applications in photodynamic therapy. A new complex containing pyrazine (pz) as the ligand trans to $N(O)SO_3^-$was synthesized by reacting the precursor*trans*-$[Ru(NH_3)_4(pz)(NO)](BF_4)$ with sodium sulfite in aqueous solution. The resulting complex*trans*-$[Ru(NH_3)_4(pz)(N(O)SO_3)](PF_6)$ was characterized by UV-Vis, FT-IR, and ^1H NMR spectroscopy. Stability studies, reaction with OH^-, and determination of the pK_a of the coordinated $N(O)SO_3$ ligand were performed. The IR spectrum of the complex showed an NO stretching band at 1942 $cm^{-1}$for the nitrosyl precursor*trans*-$[Ru(NH_3)_4(pz)(NO)](BF_4)$, which shifted to 1378 cm^{-1}upon formation of the $NOSO_3$ complex. In the ^1H NMR characterization, the ortho and meta hydrogens of the pyrazine ligand were identified by two doublets at 9.02 and 8.73 ppm, respectively. Thermal stability studies revealed pyrazine labilization, confirmed by the appearance of a free pyrazine signal at δ = 8.66 ppm in the ^1H NMR. Kinetic analysis by Uv-vis following the decay at 367 nm (T = 25 °C), resulted in the pyrazine labilization a rate constant of $k = 3.40 \times 10^{-4}\ s^{-1}$ (by ^1H NMR, $k = 4.29 \times 10^{-4}\ s^{-1}$). Reaction of*trans*-$[Ru(NH_3)_4(pz)(N(O)SO_3)](PF_6)$ with hydroxide ions (OH^-) produced the nitro complex*trans*-$[Ru(NH_3)_4(pz)(NO_2)]^+$, with a $k = 5.22 \pm 0.31\ M^{-1}s^{-1}$ (T=25°C). The pKa of the coordinated $N(O)SO_3$ ligand was determined to be 4.6, lower than that observed for related complexes. Overall, these results indicate that the ligand trans to $N(O)SO_3$ influences the stability and reactivity of this ligand.



Reactivity and stability of the trans-[Ru(NH3)4(pz)(N(O)SO3)](PF6) complex.

Agradecimentos/Acknowledgments

The authors thank FAPESP (grant no. 24/23781-2 and 2025/09383-7), CAPES, and CNPq for the financial support provided for the development of this work.

Synthesis, crystal structure, and luminescence of a heterotrinuclear TbIII-NaI β-diketonate complex

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Palavras Chave:*Lanthanide,Rare eart,Luminescence,Coordination chemistry*

Highlights

Heterotrinuclear TbIII β-diketonate complex;

Bright luminescence of TbIII complexes in the green spectral range.

Resumo/Abstract

Luminescent TbIII complexes have been investigated for applications in temperature sensors or in solid-state lighting, for instance. β-diketonate ligands such as $acac^-$ (acetylacetonate) are commonly employed as sensitizers of the TbIIIluminescence to overcome the poor molar absorptivity displayed by*f-f*electronic transitions. β-diketonate ligands normally coordinate to TbIII in a bidentate chelate mode, but in less common cases, they can also work as a bridge between metallic centers.[1] Herein, we report the synthesis of the luminescent heterotrinuclear $[Tb_2Na(acac)_6(bpy)_2]Cl$ complex (bpy: 2,2'-bipyridine) using $acac^-$ to bridge TbIII and NaIcenters. This composition was obtained by controlling the order of reagent addition. For that, $TbCl_3{\cdot}6H_2O$ (0.2600 g) and bpy (0.2001 g), both dissolved in 10 mL of methanol, were first mixed. Na^+acac^- (0.226 g) dissolved in 10 mL of methanol was added, and the solution was stirred for 4 hours. The solution was then kept undisturbed to obtain single crystals. Single-crystal X-ray diffraction reveals that the cationic complex is a heterotrinuclear specie where the two TbIII centers are connected to NaI by $acac^-$. Each TbIII is coordinated to three bidentate $acac^-$ ligands while one of the oxygens of each $acac^-$ is also coordinated to NaI, bridging TbIII to NaI. The terminal position of each TbIII is filled by the bidentate bpy ligand, leading to a coordination number of eight to TbIIIand six for NaI. Upon UV excitation, the bright green TbIII luminescence is observed owing to $^5D_4 \rightarrow {}^7F_{6-0}$electronic transitions. The luminescence arises from the well-known antenna effect played by $acac^-$, where the ligand absorbs energy and transfers it to TbIII, leading to its characteristic luminescence. Therefore, this study highlights the important role of the synthetic steps to obtain bright luminescent TbIII β-diketone complexes with uncommon stoichiometries.

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Agradecimentos/Acknowledgments

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Synthesis of a Tetradentate Schiff Base for Phosphorus Mobilization: Spectroscopic Characterization and Agricultural Potential

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Palavras Chave:*Schiff base,Chelating agents,Phosphorus,Spectroscopic characterization,Fertilizers*

Highlights

The ligand exhibited selective chelation toward metal ions, preventing phosphorus immobilization in tropical soils. Spectroscopic analyses using FTIR and UV-Vis techniques

Resumo/Abstract

Phosphorus (P) availability in tropical soils is strongly limited by the formation of insoluble phosphates with Fe^{3+} and Al^{3+} ions. This work reports the synthesis and characterization of a symmetric tetradentate chelating ligand ($C_{18}H_{20}N_2O_4$) and its metal complex, aiming to enhance P bioavailability through the selective sequestration of these interfering cations. The ligand was synthesized via Schiff condensation between 2,4-dihydroxyacetophenone and ethylenediamine. Elemental analysis (CHN) confirmed the purity and stoichiometry of the ligand (C: 64.56%; H: 6.29%; N: 8.67%). FTIR spectroscopy evidenced the formation of the imine bond through an intense ν(C=N) stretching band in the characteristic region, confirming the success of the condensation reaction. The ν(O–H) stretching band associated with the phenolic hydroxyl groups was also observed, which are essential for metal coordination. UV–Vis spectra of the complex exhibited intense absorption bands in the 210–330 nm range, attributed to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions of the conjugated system and azomethine group, in agreement with literature reports for tetradentate Schiff base metal complexes. The free ligand exhibited hydrophobic behavior, being soluble in toluene and chloroform; however, complex formation under alkaline conditions (NaOH/KOH) resulted in complete water solubility, a critical property for application in nutrient solutions. These results indicate that the synthesized system presents suitable structural, electronic, and solubility properties to act as an efficient chelating agent, representing a promising strategy for the development of smart fertilizers capable of mitigating phosphorus fixation in soils.

Synthesis of Luminescent Titanate Nanotubes Hybrids Functionalized via Ugi Reaction Coordinated to Eu^{3+} Ions for Potential Toxic Metal Sensing

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Palavras Chave:*Hybrids,Ugi Reaction,Europium,Sensor,Titanate Nanotubes*

Highlights

An Eu^{3+}-coordinated, Ugi-functionalized titanate nanotube hybrid was synthesized, exhibiting intense red emission and potential for toxic metal sensing.

Resumo/Abstract

Luminescent hybrids based on Eu^{3+} ions incorporated into functionalized TiO_2-derived nanostructures have attracted considerable attention in sensing due to their outstanding optical properties[1,2]. Unlike conventional Eu^{3+} doping, which often leads to inefficient emission, functionalization of nanomaterials with organic ligands enables effective coordination, improved energy transfer, and enhanced luminescence[1,2]. This study reports the synthesis and characterization of a luminescent hybrid based on titanate nanotubes (TiNTs) functionalized by using the Ugi reaction and subsequent coordination with Eu^{3+} ions, aiming at toxic metals sensing. TiNTs were synthesized via the alkaline hydrothermal method, followed by silanization with 3-aminopropyltriethoxysilane (APTES) to obtain TiNTs-1. This silanized material was used in an Ugi reaction with benzoic acid, cyclohexylisocyanide and benzaldehyde to form an α-aminocarboxamide derivative (TiNTs-2). The resulting product acted as a ligand for Eu^{3+} coordination, yielding the luminescent hybrid TiNTs-3. FTIR analysis provides evidence of the material formation through the shift of the deprotonated amide ν_sC=O stretching band from 1382 cm^{-1} in TiNTs-2 to 1408 cm^{-1} in TiNTs-3 (Fig. 1A). The PL spectrum of TiNTs-3 confirmed efficient energy transfer from the matrix to the Eu^{3+} center, showing a maximum emission intensity at the $^5D_0 \rightarrow {}^7F_2$ transition, highlighting the sensing potential (Fig. 1B). Otherwise, forbidden transitions are observed due to the relaxation of selection rules in the low-symmetry environment surrounding the Eu^{3+} ion. Additionally, the luminescence decay was fitted with a monoexponential model, yielding an excited-state lifetime (τ) of 0.7343 ms (Fig. 1B). TEM, TGA analysis and tests with toxic metals are being carried out to further expand the studies on the properties and morphology of the hybrid.

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[2] K. Tang et al., Opt. Mater.**2014**, 36, 1520-1524.

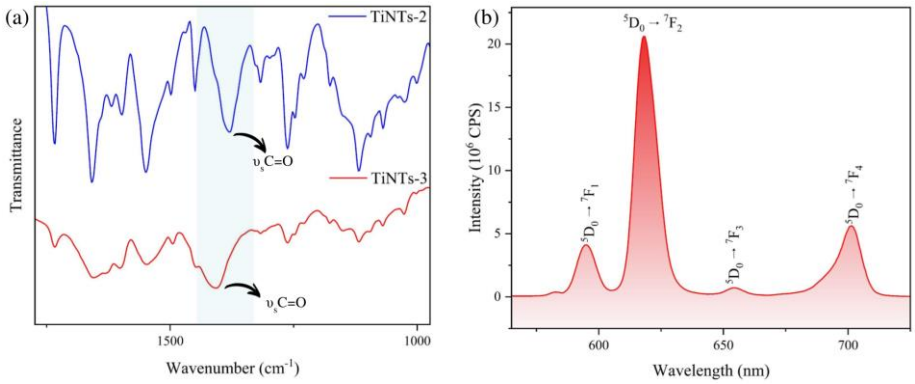


Fig. 1. (a) FT-IR spectra of the samples and (b) emission spectrum of TiNTs-3 at λex = 280 nm.

Agradecimentos/Acknowledgments

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Synthesis of NaYF4:Eu luminescent microcrystals using rare earth oxides recovered from fluorescent lamp recycling waste

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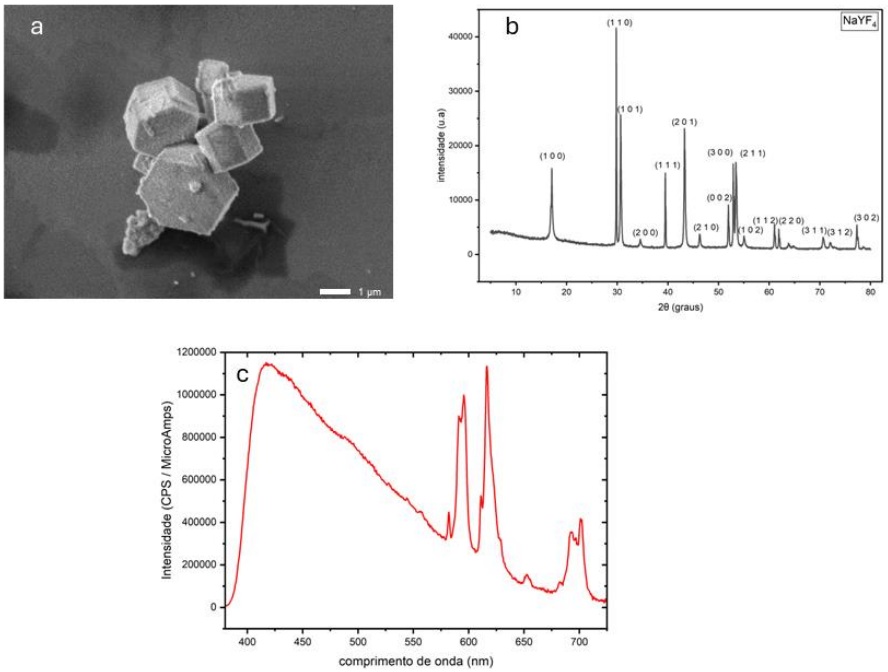
Palavras Chave:*Rare earth recycling; Y_2O_3:Eu^{3+}; $NaYF_4$:Eu^{3+}; Hydrothermal synthesis; Luminescent materials*

Highlights

Phase-pure luminescent shaped β- $NaYF_4$:Eu^{3+} microcrystals are obtained from rare-earth oxides recovered from fluorescent lamp recycling waste.

Resumo/Abstract

This study investigates the recovery of yttrium and europium from fluorescent lamp waste and their subsequent application in the synthesis of the luminescent material $NaYF_4$:Eu^{3+}, a host matrix widely recognized for its high optical efficiency and low phonon energy, particularly in its hexagonal phase (β-$NaYF_4$). Rare earth elements were initially extracted through hydrometallurgical routes involving acid pre-treatment, leaching, selective precipitation with oxalic acid, and calcination, yielding Eu^{3+}-doped Y_2O_3 oxides. Powder X-ray diffraction (XRD) analysis revealed that acid pre-treatment and oxalate precipitation conditions (pH and temperature) are critical for obtaining phase-pure Y_2O_3:Eu^{3+}. For instance, samples prepared without acid pre-treatment exhibited CaO as the major phase, while those obtained under non-optimized precipitation pH and temperature showed CaO contents higher than 10 wt% (calculated by Rietveld method from XRD data). The obtained oxides were employed as precursors for rare-earth fluoride synthesis via a microwave-assisted hydrothermal method, involving previous acid dissolution, addition of EDTA as complexing agent and precipitation with aqueous NaF solution. The obtained materials were characterized by X-ray diffraction, scanning electron microscopy coupled with EDS, and photoluminescence spectroscopy. The results indicate that acid pre-treatment and precursor precipitation conditions of the have a direct influence on the crystalline phase, morphology, and luminescent performance of the synthesized $NaYF_4$:Eu^{3+}. Higher-purity precursors [3] favor the formation of more uniform hexagonal-shaped β- $NaYF_4$:Eu^{3+}particles with enhanced Eu(III)-based emission intensity, highlighting the sensitivity of the fluoride matrix to residual impurities from the recycling process and demonstrating the feasibility of waste reuse as a sustainable source of rare earth elements for photonic applications.



(a) SEM image. (b) XRD diffractogram. (c) Emission spectrum recorded using a fluorimeter.

Agradecimentos/Acknowledgments

Authors thank CNPq (grant 407747/2022-2) and FAPESP (grant 2025/08960-0) for financial support.

Synthesis, structural characterization, and study of the magnetic properties of a pyridyl(vinyl) benzoate based dysprosium complex.

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Palavras Chave:*Dysprosium (III), Lanthanide complex, Molecular magnetism.,Dysprosium (III), Lanthanide complex, Molecular magnetism.*

Highlights

This study reports the synthesis and characterization of a dysprosium(III)-based coordination compound and investigates its magnetic properties.

Resumo/Abstract

Ligands containing carboxylate, pyridine, and vinyl groups are of significant interest due to their versatility and strong metal–ligand interactions. In particular, carboxylates can adopt multiple coordination modes, leading to diverse crystal lattice topologies depending on the metal ion and reaction conditions. Thus, this work presents a coordination compound synthesized from the reaction between the potassium {3-[2-(4-pyridyl)vinyl]}benzoate (3,4-Kpvb) and the dysprosium(III) ion. The product obtained from the reaction between 3,4-Kpvb and dysprosium nitrate hexahydrate $Dy(NO_3)_3 \cdot 6H_2O$ under magnetic stirring for 1h was characterized by Fourier-transform Infrared Spectroscopy (FTIR), elemental analysis (CHN), thermogravimetric analysis (TGA), X-ray powder diffraction and magnetic measurements. FTIR spectroscopy showed no significant differences in the C–H (trans vinyl), C=N, and symmetric COO^- stretching bands. However, for the asymmetric COO^- stretch, the shift from 1388 cm^{-1} in 3,4-Kpvb to 1401 cm^{-1} in the product indicates coordination of the ligand to the dysprosium(III) ion via the carboxylate group in a monodentate mode. According to the TGA results there was a loss of $2H_2O$ at temperatures between 110°C and 200°C. The elemental analysis results for the molecular formula $C_{42}H_{30}N_3DyO_6 \cdot 2H_2O$ where: calculated: C 57.90%; H 4.32%; N 4.74%; found: C 53.87%; H 4.08% N 4.90%. Magnetic measurements under DC and AC fields were performed on the Dy(III) complex. DC magnetic measurements showed only minor variations upon decreasing temperature. In contrast, AC susceptibility measurements, performed under zero and non-zero external DC fields, exhibited a significant increase in the out-of-phase (χ″M) signal with decreasing temperature and increasing applied DC field, suggesting that further investigations are required to confirm the presence of slow magnetic relaxation.

Agradecimentos/Acknowledgments

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Taurine and Analogous Structures as Potential Inhibitors Candidates for Adenosine-5'-phosphosufate Reductase: a Molecular Dynamics Simulation Study

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Palavras Chave:*sulfate-reducing bacteria,adenosine-5'-phosphosufate reductase,molecular docking,MD simulations*

Highlights

Evaluation of taurine analogues as inhibitors candidates to prevent H_2S-driven oil pipe corrosion. Molecular Dynamics help guide the development of enzymatic inhibitors for industrial applications.

Resumo/Abstract

Sulfate-reducing bacteria (SRB) are a type of microorganism frequently found in oil reservoirs. However, their ability to reduce SO42- to S2- via a dissimilatory pathway generate H2S during the oil exploration process which can cause pipe corrosion, plugging of the petroleum formation and serious environmental damage.1 One of the enzymes involved in the sulfate-reducing dissimilatory pathway is the adenosine-5'-phosphosufate reductase that reduces APS to sulfite and AMP, using FAD as a cofactor.2

In this context, based on previous works of our research group3, taurine and 4 other analogous structures were evaluated as potential inhibitors candidates for adenosine-5'-phosphosufate reductase through docking and molecular dynamics simulations. First, each ligand was submitted to an energy minimization through DFT calculations in the Gaussian 16W program. The change and correlation functional wB97XD were used associated to the basis set 6-311G(d, p).

Docking simulations were executed with the AutoDock Vina 1.1.2 software for the APS with optimized binder structures. The results showed that in all cases the best position was pose 1 based on its lower energy (Table 1). The molecular dynamics simulations were performed using the GROMACS 2019 package with force field CHARMM36 and the parameters obtained in our previous work4. So far, we have evaluated the RMSD, clusterization (Table 1) and hydrogen bonds (Table 2) for all ligands. Currently, more detailed studies are being conducted to determine if these molecules could be good candidates for adenosine-5'-phosphosufate reductase inhibition.

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Table 1: Molecular docking and Molecular dynamics results.

	Molecular docking		*Molecular dynamics*	
Ligands	E_{bin} (kcal/mol)	Distance S – FAD (Å)	RMSD (Å)	Cluster distance of S – FAD (Å)
APS	-9.9	11.7	2.94 ± 0.87	6.9
Taurine	-4.0	3.8	4.32 ± 1.24	5.5
Cl-Taurine	-4.1	5.5	1.55 ± 0.33	10.7
Isethionic Acid	-3.5	5.3	2.27 ± 0.31	6.5
Homotaurine	-3.9	5.1	3.48 ± 0.42	8.1
Hypotaurine	-3.3	3.4	6.42 ± 3.07	17.3

Table 2: Most stable H-Bond calculated (percentage > 40%)

Ligands	APS	Taurine	Cl-Taurine	Isethionic Acid	Homotaurine	Hypotaurine
Amino Acid Residue	ARG2265 VAL2273 GLY2274	GLN2145 ASP2361	TRP2234 VAL2273 GLY2274 ALA2275	ARG2265 HSE2398	GLN2145 ALA2275 GLU2141 ASP2361	ASP2361 ASP2364

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Temperature-dependent photoluminescence properties of Ca2MgSi2O7:Eu2+

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Palavras Chave:*Åkermanite,Lanthanide,X-Ray Diffraction,Photoluminescence Spectroscopy,Bandshift*

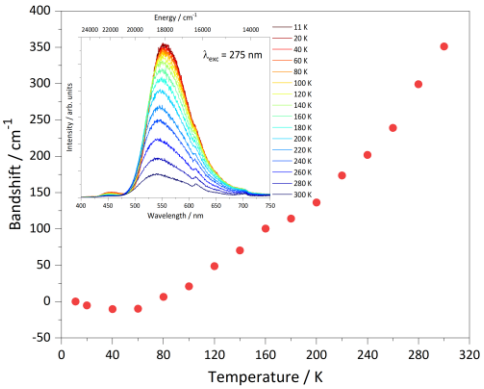
Highlights

Eu^{2+}-doped $Ca_2MgSi_2O_7$ optical proprieties were studied. A yellowish-green emission dominates the spectrum under UV excitation. The centroid shifts to higher energy as temperature rises from 80-300 K.

Resumo/Abstract

Lanthanide-doped phosphors exhibit notable optical properties due to the incomplete 4*f*shell. Europium is one of the most widely used lanthanides, with applications ranging from displays and lighting to security features for passports and banknotes. Eu^{3+} luminescence consists of narrow bands in the orange-red spectral region under UV excitation. On the other hand, Eu^{2+}, which presents a stable half-filled $4f^7$ configuration, possesses a completely distinct luminescence pattern. Owing to the strong crystal-field influence on the more external 5*d*orbitals, the $4f^65d^1$configuration becomes highly sensitive to the chemical environment. As a result, Eu^{2+} emission spectra commonly show a broad band with a maximum that can range from the long-wavelength UV to near-infrared. This ion can be stabilized in suitable host that offer an appropriate site size and preferably an isovalent substitution.

The host matrix chosen, $Ca_2MgSi_2O_7$, belongs to the tetragonal $P\bar{4}2_1m$ space group. Among the available sites, only the eightfold-coordinated Ca^{2+} site can accommodate Eu^{2+} to substitute, being the dopant 11.6% bigger than the alkaline earth metal ion. The $(Ca_{0.99}Eu_{0.01})MgSi_2O_7$ was synthesized through solid-state reaction at 1325 °C for 8 hours in a reducing CO atmosphere produced by activated charcoal. XRD confirmed crystallinity and phase formation. Photoluminescence spectroscopy revealed the presence of unreduced Eu^{3+}. Furthermore, the material presents a persistent luminescence with a biexponential decay curve with calculated lifetimes of 0.649 and 6.91 s at 275 nm excitation, in addition to 0.04 and 0.07 quantum yield under 275 and 393 nm excitation, respectively. The low quantum-yield values may arise from energy transfer to Eu^{3+} or from trap filling, which contributes to the afterglow and competes with the emission during measurement. Optical measurements from 11-300 K indicated thermal quenching (T_{50}) at 246 K and a blueshift from 80-300 K can be attributed to lattice expansion.



Bandshift versus temperature, with the inset presenting emission spectra in the 11–300 K range

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Tuning chirality and antennae effect on heteroleptic coordination polymers containing EuIII towards bright CPL emission

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Palavras Chave:*Lantanídeos, CPL, polímeros de coordenação, luminescência,Lantanídeos,CPL,Polímeros de coordenação,Luminescência*

Highlights

Lanthanide CPL emitting coordination polymers; chiral camphor's boost g_lu_m, antennae ligands enhance quantum yields, new bridge chiral ligands; heteroleptic complexes can reach high CPL brightness.

Resumo/Abstract

Circularly polarized luminescence (CPL) is increasing in interest owing to its potential applications in digital displays, quantum communication and anti-counterfeiting technologies. CPL refers to a state of polarization of the light in which the components of the electric field are phased off by 90°. Upon interaction of unpolarized light with naturally oriented matter, like chiral compounds, circularly polarized emission may be observed. LnIII ions are well-known for their unique luminescent properties such as long emission lifetimes, narrow emission bands and high purity of color. In special, EuIII shows a set of electronic transitions that are ideal for use in circularly polarized emitters. In CPL emitting complexes, it is fundamental to ensure chirality in the framework while maintaining high absorption and emission quantum yields. Most often this may be achieved by tuning chiral and sensitizing ligands in a heteroleptic coordination structure. In this work, four CPL emitting coordination polymers containing EuIII have been synthesized. Two of them were prepared with one of the chiral camphors: (+)-3-(trifluoroacetyl)camphor ((+)-facam) or 3-heptafluorobutyryl-D-camphor ((+)-hfbc) as main ligands, and the bridge ligand, ethane-1,2-diylbis(diphenylphosphine oxide) (dppeo), known for sensitizing the EuIII emission. The other two one contain the antennae thenoyltrifluoroacetone (tta) main ligand and one of two novel chiral bridge ligands ([[(2*R*,3*R*)-3-diphenylfosforylbutan-2-yl]-phenylphosphoril]benzene) ((*R*)-chiro) or ([[(2*S*,3*S*)-3-diphenylfosforylbutan-2-yl]-phenylphosphoril]benzene) ((*S*)-chiro). Their formation was ensured by FTIR measurements. The emission and absorption spectra, as well as the emission lifetime of the compounds match the expected for EuIII. The CPL emission spectra were measured, and g_lu_m values are comparable to similar species described in the literature. Further testing may lead to improvement of those compounds as CPL emitters.

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Ultrasound stimulus for nitric oxide release from nitrosyl ruthenium complex: influence of RuII—NO+ linkage

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Palavras Chave:*nitrosyl ruthenium complex, nitric oxide, ultrasound.,nitrosyl ruthenium complex, nitric oxide, ultrasound.*

Highlights

Nitrosyl ruthenium(II) complexes release nitric oxide under ultrasound stimulation; NO release efficiency depends on the RuII–NO^+ linkage and ligand environment.

Resumo/Abstract

Nitrosyl ruthenium(II) complexes are widely studied for their ability to release the nitric oxide (NO), which has therapeutic potential and is used in cancer treatment, primarily through photodynamic therapy (PDT). This work proposes the use of ultrasound stimulus as an alternative to light in PDT, for NO release from nitrosyl ruthenium(II) complexes. The position of the IR vibrational peaks for the N≡O for the complexes $[RuIICl_3NO]$, $K_3[RuIICl_5NO]$ and $[RuII(bdq)(tpy)NO]^{3+}$ are on the order of: 1850 cm^{-1}, 1880 cm^{-1} and 1895 cm^{-1}. The release of nitric oxide (NO) from ruthenium complexes was quantified using the Griess spectrophotometric method. The samples, containing solutions of the complexes at a concentration of 50 µmol L^{-1}, were subjected to four consecutive cycles of ultrasound (US) irradiation, each lasting 15 minutes, operating in continuous mode, at a frequency of 3MHz and a power of 2.5W cm^{-2}, totaling 1 hour of exposure. For the complexes $[RuIICl_3NO]$ and $K_3[RuIICl_5NO]$, NO release was quantified directly using the nitric oxide detection method, by monitoring the absorbance at $\lambda_{496\ nm}$. The concentrations of NO released were 16.8 and 8.6 µmol L^{-1} for the complexes $[RuIICl_3NO]$ and $K_3[RuIICl_5NO]$, respectively. In contrast, for the complex $[RuII(bdq)(tpy)(NO)]^{3+}$, NO release was evaluated indirectly through the quantification of nitrite (NO_2^-), formed by the acid-mediated conversion of nitric oxide, by measuring absorbance at $\lambda_{540\ nm}$. The nitrite concentrations determined were 6.0 µmol $L^{-1}$for the complex. Upon light stimulus, the presence of a stronger RuII→NO^+back-bonding interaction, which facilitates the release of NO from the ruthenium(II) complexes. However, under ultrasound stimulus the longer RuII—NO bond length has been demonstrated the influences in the NO release.

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Uso de agentes funcionalizantes/dopantes na produção sustentável de Carbon Dots de efluentes suínos

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Palavras Chave:*Carbon Dots,C-dots funcionalizados,Síntese hidrotermal,Nanomateriais sustentáveis.,funcionalização,dopagem Nanomateriais,sustentabilidade*

Highlights

The sustainable use of swine effluents in the synthesis of luminescent nanocarbons, which can be functionalized and doped to enhance their optical properties.

Resumo/Abstract

Carbon quantum dots (PQCs), also known as Carbon Dots (C-dots), are luminescent nanomaterials composed mainly of carbon that exhibit adjustable photoluminescent properties, high chemical stability, good solubility in aqueous media, low toxicity and biocompatibility. These characteristics make these materials promising for various applications, such as sensors, bioimaging and optical devices. Furthermore, C-dots can be synthesized from organic waste, which enables sustainable routes aligned with the principles of green nanotechnology. In this context, effluents from pig farming have potential for reuse, as they are rich in organic matter and carbonaceous compounds, and can act as precursors in the synthesis of these nanomaterials. In this work, the synthesis of C-dots was carried out from swine farm effluents through a bottom-up route, using a microwave-assisted hydrothermal process. The synthesis was carried out in closed Teflon reactors, at temperatures of up to 210 °C for 1 hour and 30 minutes, using 20 mL of effluent without prior treatment. Boron, urea and sulfur were used as functionalizing/doping agents, with the aim of modifying the optical properties of the materials obtained. Characterization was carried out using UV-Vis spectrophotometry (200–900 nm) and fluorescence spectroscopy. All samples showed luminescent emission under ultraviolet radiation, confirming the formation of C-dots. Samples excited at 337 nm showed luminescence in the blue region of the visible spectrum (400–550 nm), with an emission maximum at approximately 450 nm. The boron-doped sample showed higher emission intensity compared to the other samples. The UV-Vis spectra showed bands between 200 and 300 nm, associated with the π–π* and n–π* transitions. The results indicate that the doping/functionalizing agents increase the luminescent effect of the samples, without the occurrence of band shift, suggesting the functionalization of the samples.

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Reunião Anual da Sociedade Brasileira de Química

MAT - Química de Materiais

ACRYLATION OF MACAW OIL FOR 3D PRINTING APPLICATION: OPTIMIZATION OF ACRYLIC ACID AMOUNT IN THE REACTION

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Palavras Chave:*Renewable polymers,Vegetable oil,Photopolymerization,3D printing*

Highlights

The acrylation reaction of macaw oil was optimized, and the best system was used for application in the 3D printer by photopolymerization.

Resumo/Abstract

Polymers are still mostly obtained from non-renewable sources, which drives the search for sustainable alternatives, such as chemically modified vegetable oils. Macaw oil stands out because it is not intended for food, has wide availability in Brazil, and presents specific characteristics for obtaining photosensitive monomers. This work aimed at the epoxidation and subsequent acrylation of macaw oil, focusing on optimizing acrylation synthesis, to produce a renewable acrylic monomer for applications in photopolymerization and 3D printing. The oil was initially epoxidized following the method described in the literature and then acrylated using different molar proportions of acrylic acid and reaction times. The conversion of epoxy groups was determined by titration, and the best-performing system was characterized by FTIR, TG-DTA, and DSC. The monomer with the highest conversion was evaluated as a resin as a photocurable resin in 3D printing. Epoxidation was proven at 64.4% conversion of double bonds. The reaction of acrylation showed greater conversion at a 1:1.1 molar ratio between epoxide and acrylic acid groups, at a reaction time of 24 hours, reaching 78.1% conversion. Thermal analyses indicated thermal stability of 181.0 °C for the monomer and 213.0 °C for the polymer obtained after photopolymerization. FTIR spectra confirmed the expected structural modifications, where 1635 cm^{-1} bands corresponding to the C=C bonds of alkenes present in the structure of vegetable oils disappeared in the acrylated oil spectrum. The optimized monomer enabled successful 3D printing, and the resulting polymers exhibit possible luminescent properties in UV light (365 nm). These results indicate that macaw oil is a promising raw material for the synthesis of renewable acrylic monomers, allowing thermal performance similar to that described in the literature, with reduced reagent consumption, making the process more economical and sustainable.

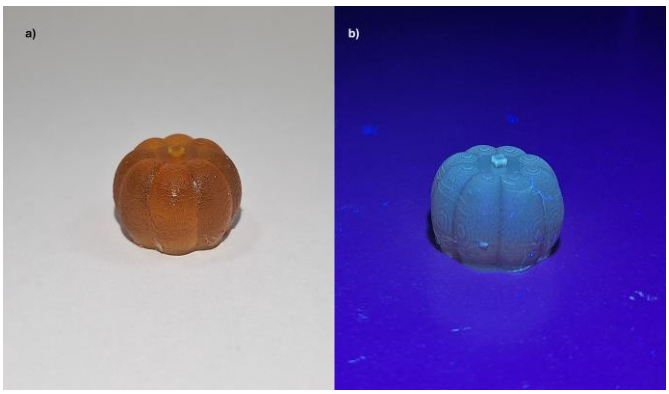


Figure 1: 3D-printed polymer from acrylic monomer under (a) ambient and (b) UV light.

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Activated carbon with ultrahigh surface area for high-pressure CO2 capture

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Palavras Chave:*avocado pit,activated carbon,high-pressure adsorption,pressure swing adsorption,porosity*

Highlights

- Ultrahigh-area activated carbon from avocado pit (3400 m^2 g^{-1});
- CO_2 uptake ~21 mmol g^{-1} at 20 bar and 25°C;
- Adsorption stability over 5 cycles.

Resumo/Abstract

High–surface-area activated carbons were prepared from avocado pit–derived char by KOH activation, targeting scalable CO_2 adsorbents from an abundant agro-waste. The precursor was carbonized and chemically activated by varying the carbonized:KOH mass ratio to 1:3 (AC1), 1:4 (AC2) and 1:5 (AC3), followed by thorough washing to remove inorganic residues and drying. N_2 adsorption–desorption at 77 K indicates that the*in natura*precursor and the carbonized sample are essentially nonporous, whereas activation generates a micro network with steep uptake at low p/p_0 and increased adsorption capacity across the full pressure range. The porous texture is highly ratio-dependent: AC1 reaches SBET=954 m^2 g^{-1} (VT=0.57 cm^3 g^{-1} and D_p = 2.39 nm), AC2 attains an ultrahigh SBET=3400 m^2 g^{-1} (VT=1.72 cm^3 g^{-1} and D_p=0.92 nm), and AC3 shows SBET=1706 m^2 g^{-1} (VT=1.37 cm^3 g^{-1} and D_p=1.37 nm), suggesting that excessive KOH loading can promote pore widening and partial structural collapse, reducing accessible surface area. SEM of AC2 reveals a sponge-like carbon matrix with abundant perforations, fractured walls and interconnected cavities, consistent with the high pore volume. Owing to its superior textural parameters and predominance of narrow pores favorable to CO_2 packing, AC2 was selected for high-pressure CO_2 capture, delivering ~21 mmol g^{-1} at 20 bar and excellent recyclability over five adsorption/desorption cycles (retention >95%) (Fig. 1). Overall, controlling the KOH activation ratio enables the conversion of avocado pits into ultrahigh-surface-area carbons with tunable microporosity and robust performance under high-pressure CO_2 adsorption conditions. The trend matches KOH activation chemistry: intermediate loading maximizes microporosity, whereas over-activation can widen pores and weaken the framework. In AC2, high SBET and VT indicate hierarchical porosity, where micropores provide strong CO_2 affinity, enabling stable cycling.

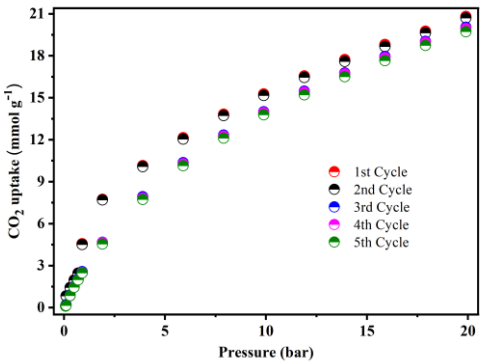


Figure 1. High-pressure CO2 uptake of AC2 over five adsorption/desorption cycles.

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Active Biodegradable Dressings Based on a Natural Polymer Incorporated with Beeswax and Essential Oil for Wound Healing Applications

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Palavras Chave:*sodium alginate,surface hydrophilicity,contact angle,wound dressing,health field*

Highlights

New biodegradable and phytotherapeutic wound dressings were developed. Methodology enables incorporation of beeswax and essential oil into alginate-based films.

Resumo/Abstract

Conventional dressings have been replaced by more sustainable and efficient alternatives [1]. In this sense, the biopolymers stand out due to the ability to incorporate active agents [2]. The main objective of this study was to prepare alginate-based films containing beeswax and*Varronia curassavica*essential oil for advanced wound healing applications. Six different formulations were studied: sodium alginate (SA); crosslinked sodium alginate (CSA); beeswax and sodium alginate (B_SA); crosslinked beeswax and sodium alginate (B_CSA); essential oil, beeswax and sodium alginate (EOB_SA); and crosslinked essential oil, beeswax and sodium alginate (EOB_CSA). For preparation of the films, the concentration of sodium alginate was fixed at 2.0 % (w/v). The concentrations of the beeswax and essential oil were maintained at 10 % (w/w) and 0.5 % (m/v), respectively. All alginate-based matrices were obtained by casting method. The crosslinked films were obtained by using manganese chloride 1.0 % (m/v). FTIR bands at 2914 and 2870 cm^{-1} indicate symmetric and asymmetric C-H stretching of sp^3 hybridization (alkene groups) present in the films with beeswax incorporated. Band at 1730 cm^{-1} was only observed in the essential oil incorporated wound dressings. It was observed that the films had different surface hydrophilicity, with the following initial contact angle values: 56.4 ± 7.9° (SA); 54.8 ± 13.6° (B_SA); 53.5 ± 5.8° (EOB_SA); 48.0 ± 9.3° (CSA); 18.0 ± 5.1° (B_CSA); and 46. 5 ± 10.6° (EOB_CSA). It was also found that the crosslinking process prevents the disintegration of the matrices during the contact angle measurements. Based on these results, it was possible to conclude that the methodology used was efficient, allowing to obtain the active films incorporated with satisfactory hydrophilicity and great potential for wound healing applications.

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Additively Manufactured Nanocellulose–Apatite Filtration Systems for Sustainable Heavy Metal Remediation

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Palavras Chave:*Cellulose nanocrystals (CNC),3D printing,Apatite composites,Water remediation,Heavy metal removal*

Highlights

Sustainable, electricity-free water filters with Eu^{3+} luminescent monitoring for developing regions.

Resumo/Abstract

Water pollution caused by heavy metals and other toxic contaminants has become a major environmental and public health concern worldwide. Exposure to heavy metals is associated with severe diseases and is a problem particularly critical in emerging countries, where mining and industrial activities frequently occur near densely populated areas. In this context, the development of low-cost water purification technologies that operate without electricity represents an important strategy to mitigate health risks and provide accessible solutions for vulnerable communities. In this work, we report the development of nanocellulose-based composite inks containing europium-doped hydroxyapatite (HAp–Eu) particles for the fabrication of filtration devices by extrusion-based 3D printing. Cellulose nanocrystals (CNC) were obtained by acid hydrolysis and characterized by transmission electron microscopy (TEM), zeta potential measurements, and dynamic light scattering (DLS). The analyses confirmed particle s and surface charges consistent with values reported in the literature. CNC suspensions exhibited birefringence under crossed polarizers and iridescence in film form, indicating the formation of a chiral nematic organization, later confirmed by scanning electron microscopy (SEM). HAp–Eu particles were synthed by spray pyrolysis with a Ca/P molar ratio of 1.64 and characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and SEM. Printable inks were formulated by combining CNC suspensions with different HAp–Eu loadings and characterized by rheology, photoluminescence spectroscopy, printability tests, and SEM. The resulting inks exhibited suitable rheological behavior and printability, enabling the fabrication of structured 3D filtration prototypes. Furthermore, Eu^{3+} luminescence may act as a spectroscopic probe to monitor structural organization and water flow within the printed filtration structures.

Agradecimentos/Acknowledgments

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Adsorption behavior of cationic dyes by Co-, Ni-, and Zn-IRMOF-74-III in aqueous solution

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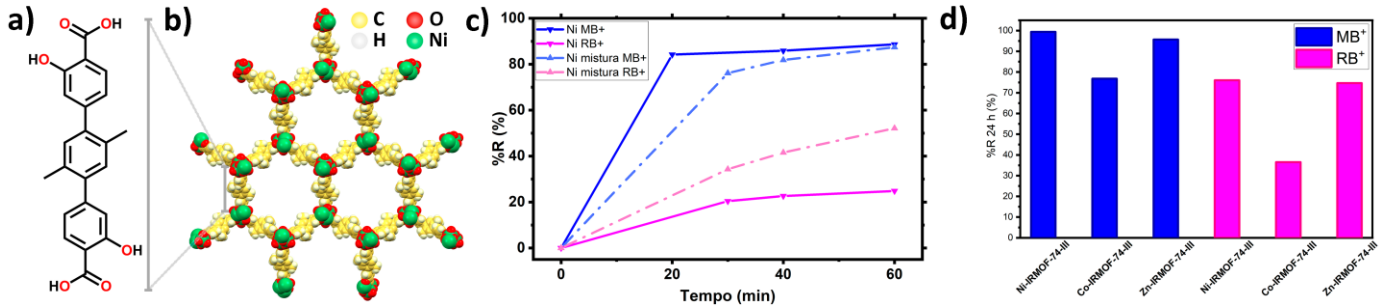
Palavras Chave:*Metal-Organic Frameworks (MOFs),dye adsorption,size selectivity,IRMOF-74,isoreticular*

Highlights

IRMOF-74-IIIexhibits size-selective adsorption of cationic dyes, favoring methylene blue (smaller) over rhodamine B regardless of the metal center, with enhanced total uptake in mixed systems.

Resumo/Abstract

The contamination of water bodies by industrial effluents containing a complex mixture of organic pollutants represents a contemporary environmental challenge. In this context, Metal-Organic Frameworks (**MOFs**) emerge as suitable materials, acting as superior adsorbents due to their controllable porosity and high surface areas, holding great potential for the selective capture of pollutants in water. In this work, we investigated the adsorption of dyes with different molecular sizes (methylene blue,**MB⁺**, and rhodamine B,**RB⁺**) using**Co**-,**Ni**-, and**Zn-IRMOF-74-III**, focusing on size-dependent adsorption behavior.**IRMOF-74-III**is an isoreticular expansion of the classic**MOF-74**, produced when the three-phenyl-ring elongated**LINKER-III**(Fig 1a) ligand is used instead of*2,5-dihydroxyterephthalic acid*. They present hexagonal honeycomb topology with unidimensional pores (Fig 1b). Single-component adsorption experiments showed that**Ni-IRMOF-74-III**removed 85% of**MB⁺**within 20 minutes, stabilizing above 90% after 1 h.**RB⁺**removal was slower, reaching only 25% after 1 h and 67% after 24 h. In binary solutions, at 30 min 76% of**MB⁺**and 34% of**RB⁺**were removed, suggesting that**RB⁺**hinders**MB⁺**adsorption while**MB⁺**synergistically enhances**RB⁺**uptake. By 60 min,**MB⁺**adsorption nearly matched single-solution levels (87%), and**RB⁺**removal (52%) remained synergistically elevated. However, at 24 hours,**MB⁺**removal exceeded 90% while**RB⁺**dropped to 28%, indicating the release of**RB⁺**back into the solution to favor**MB⁺**uptake, thus confirming selectivity for**MB⁺**.Notably, the total uptake is higher in mixed solutions than in single-component systems, summarized in Fig 1c. This adsorption behavior was consistent across different metal centers in the**IRMOF-74-III**series, indicating that the metal center does not significantly influence dye removal efficiency (Fig 1d).**Zn-IRMOF-74-III**follows the adsorption profile of**Ni-IRMOF-74-III**, while,**Co-IRMOF-74-III**presents lower efficiency.



a) LINKER-III; b) Ni-IRMOF-74-III; c) Dyes adsorption evolution; d) Maxima dye removal for each MOF.

Agradecimentos/Acknowledgments

The authors are grateful to the funding agencies FAPEMIG (APQ-05311-23 and APQ-01948-22), CNPq (420443/2018-5), and CAPES for financial support through research grants and scholarships; and to NEPs-DQ for the infrastructure.

Advances in CuInGaS2 Quantum Dot Sensitized Solar Cells

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Palavras Chave:*Quantum Dots, Colloidal synthesis, CIGS, Solar Cells, Ligand Exchange,Quantum Dots,Colloidal synthesis,CIGS,Solar Cells,Ligand Exchange*

Highlights

Colloidal synthesis of $CuInGaS_2$ QDs Ligand exchange: 1-DDT, MPA, and TGA Development of a QDSSC sensitized by QD CIGS PCE of 4.6% for CIGS@TGA

Resumo/Abstract

The growing demand for energy has led to an increased search for renewable energy sources, such as solar cells. To fully utilize this energy source, it must become more economical and efficient. Therefore, research into the development of quantum dots (QDs) sensitized solar cells (QDSSCs) is being conducted. Among the different QDs, those made of $CuInGaS_2$ (CIGS) stood out in second-generation photovoltaic applications, with significant power conversion efficiency (PCE) values, due to their excellent optoelectronic properties, with a direct bandgap that can be adjusted in the range of 1.5 eV < Eg < 2.53 eV depending on the gallium concentration, and for being free of heavy metals. However, studies on the colloidal phase are still scarce. In this work, QDSSCs sensitized by CIGS QDs, synthesized via hot injection, and deposited on TiO_2 semiconductor by immersion were investigated, followed by passivation with ZnS using the SILAR method. Initially, the CIGS PQs were linked to 1-dodecaanethiol, requiring a ligand exchange, to 1-mercaptopropionic acid (MPA) and thioglycolic acid (TGA), allowing dispersion in aqueous medium. Infrared spectroscopic measurements indicated the absence of the thiol group band, which is responsible for anchoring to QD, and the displacement of the carboxylic group bands, indicating effective exchange. Based on the diffractograms, the structure of the CIGS was not affected during the ligand exchange. Through electrical characterization, the photoanode sensitized by QD CIGS@TGA presented higher values of Jsc (14.74 mA/cm²) and Voc (0.55 V) than the MPA ligand. Although the TGA binder exhibited lower resistance (98 Ω) compared to MPA (326 Ω), it compensated for the more energetically favorable electronic injection and QD charging, achieving a higher PCE of 4.6% versus 2.68% for CIGS@MPA. These devices remained stable during the chronoamperometry studies. The research conducted indicates that these materials have potential for energy applications.

Agradecimentos/Acknowledgments

This work was supported by FAPEMIG, CNPq, FINEP, and CAPES.

A lipid-based liquid system for controlled release of the pheromone methyl 2,6,10-trimethyltridecanoate: formulation and release profile

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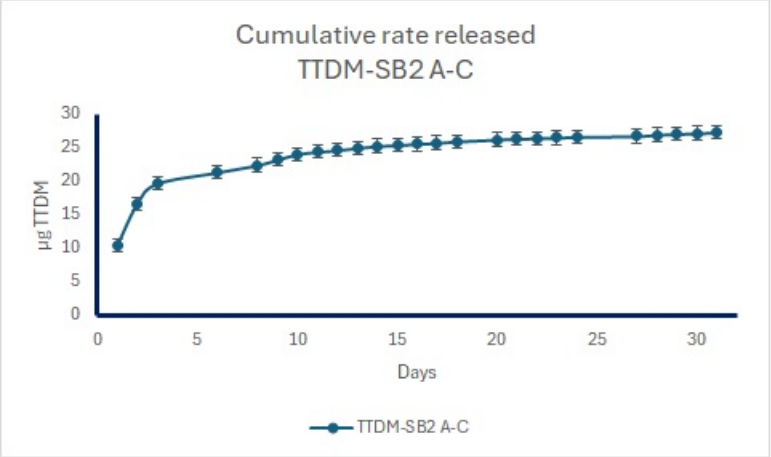
Palavras Chave:*Nanoemulsion,Lipid-based formulation,Controlled release,Pheromone delivery,Release kinetics*

Highlights

A lipid-based nanoemulsion was engineered as a carrier for pheromone delivery. The biodegradable lipid carrier shows potential for agricultural applications.

Resumo/Abstract

The use of pheromones in integrated pest management (IPM) has been progressively increasing across several crops, particularly those with high added value, such as fruits and vegetables. This study aims to evaluate an emulsion-based formulation containing soybean oil and the pheromone methyl 2,6,10-trimethyltridecanoate, the main compound involved in the chemical communication of the stink bug*Euschistus heros*.
A polymeric lipid carrier is being evaluated as a matrix for the controlled release of the compound, with the aim of increasing its efficiency and prolonging its action in the agricultural environment. The aim is to use low-cost, biodegradable carriers with minimal environmental impact.
The release rate of the pheromone from the nanoemulsion was evaluated through daily collection of volatiles over a period of 30 consecutive days. The obtained extracts were analyzed by GC-FID to quantify the amount of pheromone emitted from the emulsion on a daily basis. The release mechanism will be determined by fitting the data to the Korsmeyer–Peppas mathematical model. Preliminary field trials in soybean experimental areas demonstrated a significantly higher number of female stink bugs on soybean plants treated with the emulsion compared to untreated areas.



Cumulative rate released TTDM-SB2 A-C

Agradecimentos/Acknowledgments

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α-Borophene-Based 2D Nanomaterials: Synthesis and Characterization for Next-Generation Energy and Detection Technologies.

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Palavras Chave:*Boron,Borophene,Sonochemical exfoliation process,Semiconductor applications,2D Materials*

Highlights

α-Borophene exhibits high sensitivity for chemical and electrochemical detection. α-Borophene-based 2D materials emerge as promising platforms for advanced technologies.

Resumo/Abstract

Borophene, a 2-dimensional allotrope of boron, has emerged as a promising material for next-generation energy technologies due to its high electrical conductivity, mechanical strength, and thermal stability. Unlike other 2D materials, borophene exhibits rich polymorphism and multicenter bonding, enabling tunable electronic and electrochemical properties. In this work, crystalline boron (Sigma-Aldrich®) was fragmented and subjected to ball milling for 2 h at 300 rpm, followed by liquid-phase exfoliation in*N,N*-dimethylformamide. The dispersion was sonicated, centrifuged to remove non-exfoliated particles, and dried at 60 °C. UV–Vis spectroscopy revealed a characteristic absorption peak at approximately 190 nm, confirming borophene formation. Raman spectroscopy showed vibrational modes at 116.8, 157.3, 330, 408, 702.6, and 805 cm^{-1}, consistent with the α-borophene phase and distinct from other polymorphs. X-ray diffraction confirmed the crystalline nature of the material, indicating an anorthic crystal system with space group*P1*. Electrochemical performance was evaluated by cyclic voltammetry using bare and borophene-modified glassy carbon electrodes in a solution containing 10 µM $K_3[Fe(CN)_6]$ and 0.1 mol L^{-1} KCl. The modified electrode showed enhanced anodic and cathodic currents, indicating improved electron-transfer kinetics attributed to the high conductivity and large surface area of α-borophene. These results highlight the potential of borophene as a functional platform for energy-related and electrochemical applications.

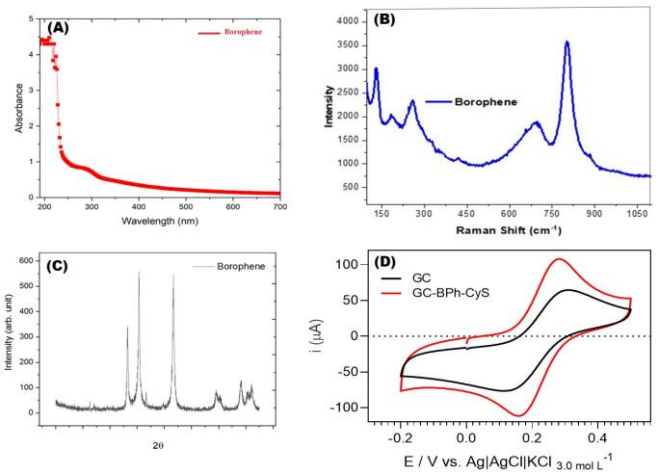


Fig. (A) UV spectroscopy analysis in DMF (B) Raman spectra (C)XRD pattern (D) Cyclic voltammograms

Agradecimentos/Acknowledgments

This research was supported by the CARREFOUR Group, CAPES (Finance Code 001), and CNPq (projects 400913/2023-2 and 404139/2022-1), with additional support from the Graduate Program in Chemical Engineering at UFRN (PPGEQ/UFRN).

Aplicação de nanomateriais de óxido de cobre(I) como sensores eletroquímicos para monitoramento de glifosato em efluentes

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Palavras Chave:*síntese de nanopartículas, caracterização, glifosato e efluentes,nanopartículas de óxido de cobre(I), síntese de nanopartículas, caracterização, glifosato e efluentes,nanopartículas óxido de cobre(I),síntese de nanopartículas,caracterização,glifosato,efluentes*

Highlights

Síntese, caracterização e aplicação de nanopartículas de Cu2O para a determinação de glifosato. Os resultados mostraram uma boa sensibilidade para concentrações abaixo do limite permitido pela ANVISA

Resumo/Abstract

O Brasil apresenta uma produção agrícola expressiva e se destaca como exportador de*commodities*no mercado global. Para acompanhar a demanda, o uso de defensivos agrícolas tem crescido. Visto que muitos desses compostos podem ser danosos à saúde humana, torna-se necessária uma fiscalização rigorosa em relação à sua aplicação. Um dos agrotóxicos mais utilizados no país é o glifosato que tem sua concentração limite regulada pela ANVISA e estabelecida em 0,5 µg/L. Assim, torna-se necessário o desenvolvimento de métodos analíticos sensíveis e de baixo custo para sua detecção. O objetivo deste trabalho consistiu na síntese, caracterização e aplicação de nanopartículas (NPs) de óxido de cobre(I) como eletrodo modificado para a determinação de glifosato. As NPs foram obtidas utilizando glicose como agente redutor, resultando em um sólido vermelho-amarronzado. A caracterização foi realizada por espectroscopia de absorção UV-Vis, difração de raios X (DRX) e microscopia eletrônica de varredura (MEV). No espectro UV-vis, observou-se uma banda entre 590-640 nm, característica das NPs de Cu_2O. No DRX, indicou-se que o material possui um tamanho médio cristalino próximo a 30 nm (2θ = 42,6º, λ=1,786Å), já no MEV, observa-se uma superfície com características esféricas com formação de aglomerados. As NPs foram incorporadas a uma pasta de grafite e Nujol em proporções variando de 0 a 75%. Avaliou-se o desempenho eletroquímico por meio de voltametria cíclica em uma célula de três eletrodos: trabalho (modificado com NPs), referência (Ag/AgCl) e auxiliar (Pt). O uso de ferricianeto de potássio como padrão analítico permitiu identificar a composição do eletrodo que conferiu a melhor sensibilidade para utilização na construção das curvas com diferentes concentrações de glifosato. Os resultados mostraram um coeficiente de correlação superior a 0,9, apresentando uma boa sensibilidade para detectar concentrações abaixo do limite permitido.

Agradecimentos/Acknowledgments

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Application of solubility theories in the development of a PLA/Carbon Black composite for the development of 3D electrochemical sensors.

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Palavras Chave:*Solubility theories, Lab-made filaments, 3D electrochemical sensors*

Highlights

Use of less toxic solvents for creating PLA-Carbon Black composite filament for 3D printing of electrochemical sensors.

Resumo/Abstract

The development of conductive Polylactic Acid (PLA) filaments via the solvent method often relies on toxic or restricted solvents. This study utilizes cohesive energy density, expressed through Hildebrand and Hansen solubility parameters, to identify safer alternatives for producing PLA and Carbon Black (CB) composites. Applying solubility theories, the geometric method in a Teas graph and Relative Energy Difference proposed a mixture of acetic acid and dichloroethane (3:1 v/v). This mixture enabled the creation of a flexible, electrically conductive PLA/CB filament (59.3 S m^{-1}) composed of 56.5% PLA, 30.4% CB, and 13.0% castor oil, which acts as a plasticizer to ensure flexibility. Raman spectroscopy confirmed effective CB incorporation, with characteristic bands identified at 2950 cm^{-1} in PLA (Figure 1-A), and at 1330 and 1580 cm^{-1} (Figure 1-B) for the PLA/CB composite (Figure 1-C). Visual representations of the materials are provided in Figure 1- A, B and C, with a magnified Raman spectrum shown in Figure 1-B. To demonstrate the applicability of this filament in electrochemical analyses, a 3D device was developed and subjected to cyclic voltammetry. As shown in Figure 1-D, the presence of the electrochemical probe $[Fe(CN)_6]^{3-/4-}$, (red curve) yielded well-defined oxidation and reduction peaks compared to its absence (black curve), evidencing efficient charge transfer at the electrode-solution interface. These results confirm that the developed filament possesses adequate conductivity and electrocatalytic activity, consolidating it as a viable and low-cost alternative for prototyping high-performance 3D electrochemical sensors.

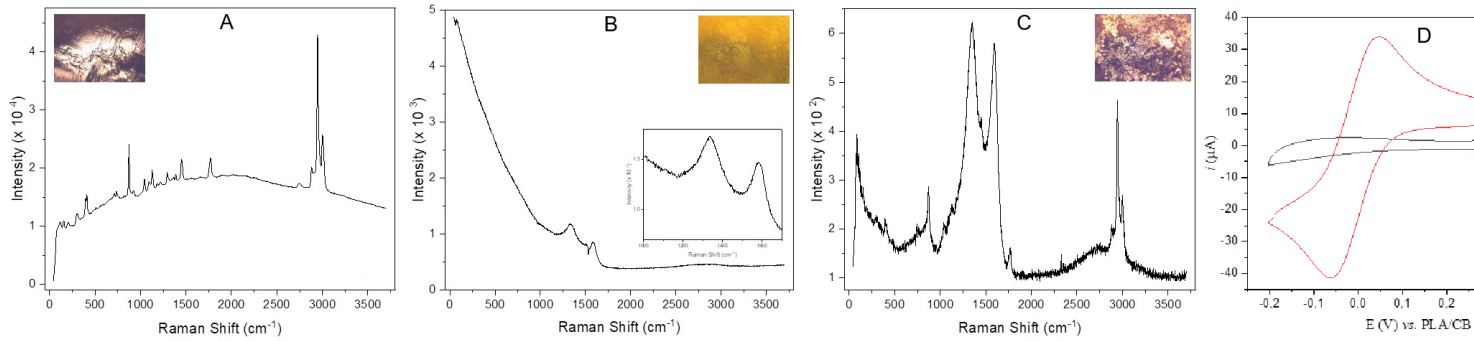


Figure 1: Raman: (A) PLA, (B) CB, (C) PLA/CB. (D) Cyclic voltammetry.

Agradecimentos/Acknowledgments

UFSJ; DCNAT; FQMAT; NEEM -UFJF; INCT-CEMAR; CNPq; CAPES and FAPEMIG

APTES loading controls structural organization in siloxane-based hybrid polyhydroxyurethanes obtained from CO2-derived cyclic carbonates.

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Palavras Chave:*Polyhydroxyurethanes,CO2-based polymers,Hybrid organic-inorganic materials,Siloxane-based polymers,Non-isocyanate polyurethane.,Polyhydroxyurethanes,CO2-based polymers,Hybrid organic-inorganic materials,Siloxane-based polymers,Non-isocyanate polyurethane.*

Highlights

APTES tunes PDMS-PHU network connectivity: gel fraction increases (33–71%) and SAXS shows a broad peak at q≈0.164 $Å^{-1}$ (d≈3.8 nm) with amorphous WAXS.

Resumo/Abstract

CO_2 fixation into cyclic carbonates is an attractive route to more sustainable polymer networks. Here, a telechelic bis(cyclic carbonate)-terminated polydimethylsiloxane (CCPDMS) was prepared by CO_2 cycloaddition to diglycidyl ether-terminated epoxidized PDMS and converted into siloxane-based polyhydroxyurethanes (PHUs) by aminolysis with 1,2-cyclohexanediamine (CID) and 3-aminopropyltriethoxysilane (APTES). Formulations F1–F8 were obtained with fixed CCPDMS and CID (1 mmol each) and varying APTES loading (0.20–0.70 mmol). FTIR-ATR confirmed cyclic carbonate consumption and urethane/hydroxyl formation. Solid-state ^{29}Si MAS NMR of selected compositions (F2 and F6) is dominated by the D-unit resonance of PDMS at ~−22.6 ppm, with a minor contribution near −20.0 ppm (D sub-population) and a low-intensity signal at +7.5 ppm (M-type, consistent with highly methylated/terminal siloxane environments). Notably, no resolved T^2/T^3 resonances (≈−59/−68 ppm) typical of APTES-derived polysilsesquioxanes are detected, indicating that silane hydrolysis/condensation, if present, is minor relative to PDMS and/or yields very broad, low-intensity features. Gel content ranged from 33 to 71% and increased approximately linearly with APTES, consistent with enhanced network connectivity and progressive formation of self-supporting films. SAXS/WAXS indicated predominantly amorphous and heterogeneous networks: WAXS lacked Bragg reflections, while SAXS exhibited a broad correlation peak at q≈0.164 $Å^{-1}$ (d≈3.8 nm) and a Guinier regime consistent with mesoscale inhomogeneities modulated by composition. Despite the presence of polar groups in the bulk, static water contact angles indicated hydrophobic surfaces, attributed to siloxane segment enrichment. Overall, APTES provides a straightforward compositional lever to tune insolubility and hierarchical heterogeneity in CO_2-derived PDMS-PHUs for film/coating applications.

Agradecimentos/Acknowledgments

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Bacterial Cellulose-Derived Biochar for Electrochemically AssistedFenton Degradation of Methylene Blue

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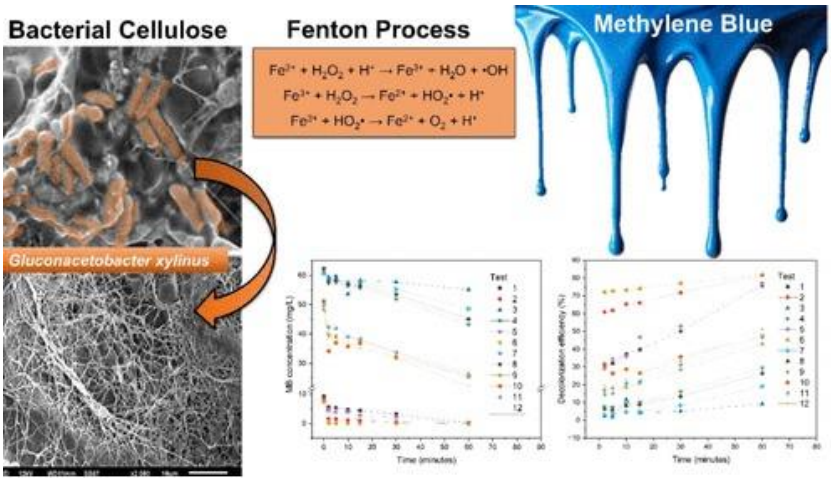
Palavras Chave:*Carbene compounds,Catalysts,Cellulose,Degradation,Dyes and pigments*

Highlights

Eco-friendly catalyst: Iron-modified bacterial cellulose biochar drives electro-Fenton degradation, reaching 82% dye removal and >50% TOC reduction in just 60 mins at varying pH levels.

Resumo/Abstract

This study explores the potential of biochar derived from bacterial cellulose (BC-derived biochar) as a catalytic support in Fenton-type processes for the degradation of methylene blue (MB) in aqueous solutions. The biochar was synthesized by modifying purified BC membranes with Fe^{2+}/Fe^{3+} ions, followed by calcination at 400 °C. The performance of three treatment approaches (electrochemical degradation, heterogeneous Fenton process, and a combined treatment integrating both methods) was evaluated. The results highlighted the superior efficiency of the combined treatment, demonstrating its potential for practical applications. A 2^3 factorial design with a central point was employed to evaluate the effects of key variables in the electrochemically assisted Fenton process: MB concentration, BC-derived biochar concentration, and reaction pH. Statistical analysis, with an R^2 value of 0.989, revealed that only the dye concentration and biochar concentration had statistically significant effects, while pH and interaction effects were negligible. Discoloration efficiencies reached nearly 80% for 10 ppm solutions at both acidic and basic pH, with a maximum treatment time of 60 min, demonstrating the versatility and effectiveness of the Fenton system in diverse media. Additionally, a kinetic study further supported these findings, with the best result fitting a first-order reaction model (R^2 = 0.984). The total organic carbon analysis confirmed the method's efficiency, showing a reduction in the organic compound by over 50% for both 10 and 55 ppm solutions. These results demonstrate that the proposed method is a promising alternative for treating MB dye and can be extended to the degradation of other organic compounds.



Biochar from bacterial cellulose for electro-Fenton dye degradation.

Agradecimentos/Acknowledgments

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Bile Salt-Carboxymethylcellulose Self-Assembly: Nanocellulose Morphology Modulates Viscoelastic Properties

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Palavras Chave:*Sodium cholate,Carboxymethylcellulose,Nanocellulose,Rheology,Hydrogels*

Highlights

Nanocellulose modulate sodium cholate-CMC gelation. CNF systems exhibit 163 times higher viscosity with elastic-dominant behavior. Potential for drug encapsulation and sustainable packaging.

Resumo/Abstract

Bile salts form supramolecular aggregates whose morphology can be modulated by polyelectrolytes and nanoparticles, yet how nanocellulose morphology influences colloidal stability and network formation remains unexplored. This study investigates structure-rheology relationships in ternary hydrogels containing 50 mM sodium cholate (NaC), 1.5% (w/v) carboxymethylcellulose (CMC), and 0.48% (w/v) anionic cellulose nanocrystals (CNC) or nanofibrils (CNF). After equilibration, NaC+CMC+CNF exhibited transparent gel-like appearance, while NaC+CMC+CNC showed cream-like consistency with turbidity (Fig 1). Flow curve analyses at 0.01 s^{-1} revealed apparent viscosities of 26.06, 381.8, and 4253 Pa.s for NaC+CMC, NaC+CMC+CNC, and NaC+CMC+CNF, respectively, representing 15 times (CNC) and 163 times (CNF) higher viscosity (Fig. 2a). Oscillatory rheology at 1 rad/s showed G'/G' ratios of 0.6, 1.4, and 3.3, respectively, with CNF achieving storage modulus ~100 Pa and elastic-dominant gel behavior (Fig. 2b). Dynamic light scattering (DLS) correlation coefficients decreased from ~0.47 for NaC+CMC to ~0.15 with CNC, and ~0.11 with CNF (Fig. 2c). Zeta potential measurements showed -26.0±0.0 mV for NaC+CMC+CNF and -17.1±0.0 mV for NaC+CMC+CNC. The multi-technique correlation reveals that higher surface charge (-26.0 mV) promotes better dispersion (lower DLS correlation ~0.11), directly enhancing network connectivity and viscoelastic properties (η=4253 Pa.s, G'/G'=3.3). This demonstrates CNF's superior performance through charge-mediated homogeneous distribution and efficient bridging between CMC chains via bile salt micelles, producing transparent gels suitable for drug delivery. Future work will investigate cationic nanocellulose interactions and film and electrospun fiber formation for potential wound healing and bioactive packaging applications.

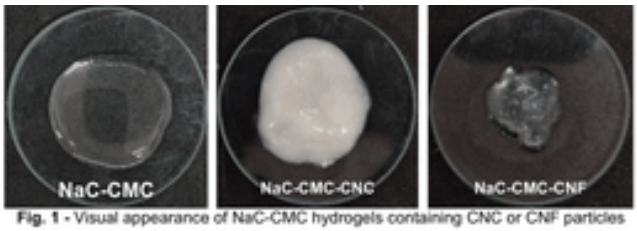


Fig. 1 - Visual appearance of NaC-CMC hydrogels containing CNC or CNF particles

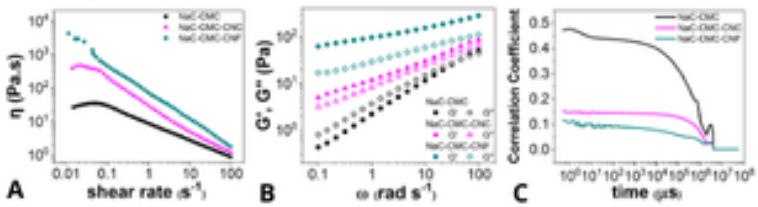


Fig. 2 - Rotational (a), oscillatory (b) rheology and DLS correlation (c) of NaC-CMC with CNC or CNF

Agradecimentos/Acknowledgments

The authors acknowledge FAPESP (Grant 24/00851-5), CNPq (Grant 141298/2024-3), UFSCar/CCA, and CNPEM for financial support and research infrastructure.

Biodegradation of renewable foams adjusted with biomass particles and biopolymers

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Palavras Chave:*Foams, Sugarcane bagasse, Eucalyptus wastes, Biodegradation kinetics, Packaging.,Foams, Sugarcane bagasse, Eucalyptus wastes, Biodegradation kinetics,Packaging.,foams,sugarcane bagasse,eucalyptus waste,biodegradation,packaging*

Highlights

Renewable foams prepared by foam-forming and oven-drying.

Foam biodegradation kinetics can be tailored, making them versatile options for green packaging.

Resumo/Abstract

Renewable foams are environmentally friendly alternatives to plastic foams used in packaging, such as expanded polystyrene (EPS). For packaging applications, renewable foams must be able to absorb mechanical energy and have biodegradation rates that match the product's shelf life. This study introduces a novel approach to producing renewable foams via foam-forming, by combining unrefined lignocellulosic particles from sugarcane bagasse (SB) and eucalyptus waste (EW), biopolymers pectin and starch, and a surfactant. The systems were subjected to mechanical agitation to incorporate air bubbles and form highly stable aqueous foams, then oven-dried to obtain solid foams, yielding materials with low density (0.07 to 0.26 g cm^{-3}) and compressive strength (0.08 to 0.27 MPa), comparable to EPS. Biodegradation was evaluated by burying the materials in compost soil in Bartha and Pramer flasks, monitoring the foam decomposition by measuring CO_2 release. The foams biodegraded at different kinetics depending on their composition, as revealed by analysis using a Gompertz model. SB foams exhibited shorter lag times (0.09 - 5.8 days) compared to EW foams (12.4 - 19.5 days). SB foams decomposed more rapidly, which can be attributed to their higher hemicellulose content (29 wt.%) and thin cell walls (< 1.5 µm). The biodegradation rate was influenced by the type of biopolymer present in the foams, with faster rates observed with starch-based foams than with pectin-based foams, as the heterogeneous branched structure of pectin hinders enzymatic access. Therefore, this work demonstrates that the biodegradation kinetics of renewable foams can be adjusted by selecting different biomass particles and biopolymers, making them adaptable for packaging products with varying shelf lives.

Agradecimentos/Acknowledgments

FAPESP through the Young Investigators Grant (23/09659-7), and the Research, Innovation and Dissemination Center for Molecular Engineering for Advanced Materials – CEMol (Grant CEPID No. 2024/00989-7). VBPS thanks the scholarship FAPESP 23/14118-5.

Biomass-derived thiol–epoxy thermosets: a comparative study with conventional systems

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Palavras Chave:*renewable monomer,thermal analysis,click-chemistry*

Highlights

From biomass to thermosets: thiol–epoxy polymers for sustainable materials chemistry

Biobased thiol–epoxy thermosets show thermal performance comparable to DGEBA while reaching 62% biobased content

Resumo/Abstract

Polymers based on thiol-epoxy, also known as thiol-epoxy click reaction, have demonstrated great potential as dynamic polymer networks (DPNs), including those derived from renewable sources.[1] Therefore, the present work aimed to produce and characterize a new thermosetting polymer with high biobased content and possible DPNs properties. For this, epoxidized macaw vegetable oil (EMWO, a Brazilian Biomass) was crosslinked with a polythiol (trimetilolpropano tris(3-mercaptopropionato), resulting in the thermosetting PMWO. For comparison, the polymerization was also carried out using the conventional epoxidized monomer diglycidyl ether of bisphenol A, resulting in the polymer PDGB. The systems were evaluated with and without catalysts. Systems using catalysts achieved global conversions of above 97% (measured by MIR) and exhibited a temperature of thermal stability (under dry air atmosphere) of approximately 230.0 ºC. Although both samples showed temperature of maximum degradation rate of around 350.0 ºC, PMWO presented a lower maximum degradation rate (6.0 % min-1) compared to PDGB (11.0 % min-1), indicating a slower degradation process for the biobased-polymer (determined by TG/DTG-DTA). Both polymers exhibited sub-ambient*Tg*: PMWO (-5 ºC) and PDGB (16 ºC). As expected, the biobased content of PMWO (62.0%) was higher than that of PDGB, which was null. Qualitative tests further indicated that PMWO exhibits characteristics of DPNs; however, additional characterization is required to better evaluate and quantify them. Based on these results, the renewable-based polymer exhibited properties mostly comparable to those of the DGEBA derivative, showing the great potential of EMWO as a monomer for covalent adaptable network-based polymeric materials. These findings contribute to the Circular Economy and align with the Sustainable Development Goals (SDGs), particularly Goal 9 (Industry, Innovation and Infrastructure) and Goal 12 (Responsible Consumption and Production).

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brazil. Processes Numbers 24/00779-2, 24/02935-1 and 24/14279-1).

Caracterização e lixiviação de rejeito arenoso de mineração de ferro por planejamento experimental visando aplicações avançadas

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Palavras Chave:*Rejeito de mineração,Sustentabilidade,Economia circular,Lixiviação ácida*

Highlights

Iron mining waste as an alternative sustainable source of silica.

Resumo/Abstract

O reaproveitamento de rejeitos da mineração tem se destacado como uma alternativa sustentável para a obtenção de materiais de alto valor agregado, contribuindo para a redução de impactos ambientais e promovendo a valorização de resíduos industriais. Nesse contexto, este trabalho teve como objetivo a caracterização e a lixiviação de um rejeito arenoso de minério de ferro, visando à obtenção de quartzo de elevada pureza. Inicialmente, o rejeito foi caracterizado por espectroscopia no infravermelho (FTIR), que revelou bandas de O-H e H-O-H, associadas à presença de água na superfície da material, além dos estiramentos Si–O. O teor médio de umidade, determinado pelo método da estufa (ABNT NBR 6457:2016), foi de 3,44%. Posteriormente, realizou-se a separação granulométrica, sendo a fração de 60 mesh caracterizada por fluorescência de raios X (FRX), difração de raios X (DRX) e espectroscopia de energia dispersiva (EDS). Os resultados de FRX indicaram que o rejeito é composto majoritariamente por SiO_2 (68,97%), seguido por Fe_2O_3 (25,45%) e Al_2O_3 (3,31%), além de MgO (1,81%) e outros óxidos em menores proporções, o que está de acordo com os resultados obtidos por EDS (Figura 1) e o difratograma de DRX que apresentou fase predominante de quartzo (SiO_2). O planejamento experimental teve caráter exploratório, permitindo compreender o comportamento do sistema e propor condições reacionais mais brandas em comparação às reportadas na literatura. Foram avaliados os efeitos da temperatura e da concentração de HCl por meio de um planejamento fatorial 2^2. Assim, a lixiviação foi conduzida utilizando solução de HCl 8 mol L^{-1}, sob refluxo a 100 ºC por 4 h, promovendo a dissolução das espécies metálicas. Nessas condições, obteve-se uma fração rica em SiO_2com aproximadamente 94% de pureza, demonstrando o potencial do rejeito arenoso de ferro como fonte alternativa de silício para síntese de materiais avançados, contribuindo para a sustentabilidade e valorização de resíduos minerais.

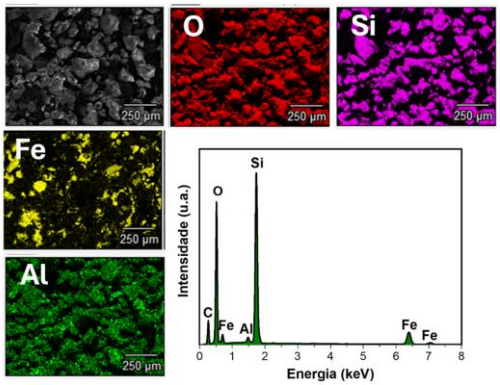


Figura 1. Mapeamento químico e espectro de EDS do rejeito arenoso de ferro.

Agradecimentos/Acknowledgments

Os autores agradecem à UFMG, à FAPEMIG e à CAPES pelo apoio financeiro, ao Grupo de Tecnologias Ambientais (GRUTAM) pela infraestrutura e ao Laboratório Nacional de Nanotecnologia para o Agronegócio (LNNA) pelo auxílio nas análises.

Carvão ativado de syzygium aromaticum impregnado com prata e cobre para aplicação no tratamento de água.

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Palavras Chave:*cravo-da-índia, poluentes emergentes, carvão ativado.,cravo-da-índia, poluentes emergentes, carvão ativado.*

Highlights

Clove-derived activated carbon represents a green and value-added route for water treatment and mitigation of emerging pollutants.

Metal-doped carbon boosts adsorption.
Clove carbon removes drug traces.

Resumo/Abstract

A crescente contaminação de ecossistemas aquáticos por poluentes emergentes, como fármacos, pesticidas, corantes e metais pesados, tem se tornado um desafio relevante para a saúde pública e para a sustentabilidade ambiental. As estações convencionais de tratamento de água e esgoto mostram-se frequentemente ineficazes na remoção desses compostos devido à sua elevada persistência química, baixa biodegradabilidade e resistência à degradação microbiana. Dentre as alternativas propostas, a adsorção em carvão ativado - CA - destaca-se por sua alta eficiência, simplicidade operacional e custo relativamente baixo. Neste contexto, este trabalho objetiva a produção de CA a partir de folhas e botões de cravo-da-índia (*syzygium aromaticum*), biomassa rica em compostos fenólicos que pode resultar em um material de elevado potencial adsortivo. O CA obtido foi submetido a ativação química com hidróxido de sódio e posterior impregnação com íons metálicos de prata e cobre, visando potencializar a interação com fármacos e as propriedades bactericidas. A caracterização do CA e do CA impregnado com metais foi realizada por espectroscopia no infravermelho por transformada de Fourier (FTIR), microscopia eletrônica de varredura (MEV), difração de raios X (DRX), análise termogravimétrica (TGA) e determinação do ponto de carga zero (pHpcz). Ensaios preliminares de adsorção foram conduzidos utilizando-se o paracetamol e dapagliflozina como contaminantes-modelo, monitorados por cromatografia líquida de alta eficiência (HPLC). Os resultados demonstraram que o CA produzido apresenta elevada capacidade adsortiva, com remoções superiores a 90% para ambos os fármacos, evidenciando a elevada interação entre os fármacos e a superfície modificada com metais do adsorvente. Os resultados confirmam o potencial do carvão de cravo como alternativa sustentável para tratar água contaminada por fármacos e poluentes emergentes

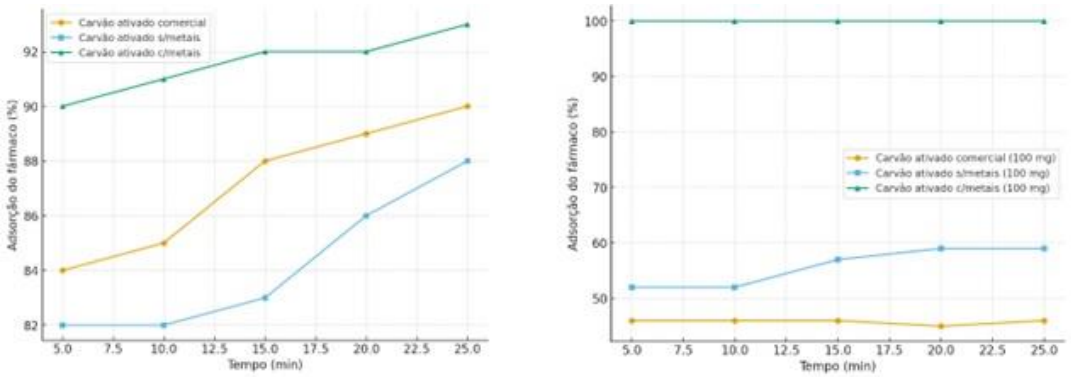


Figura 1. Adsorção de fármacos,paracetamol (esquerda) e dapagliflozina (direita), nos carvões ativos

Agradecimentos/Acknowledgments

Os autores agradecem ao GENPEC e ao GIPeFEA da UNIOESTE pela infraestrutura e apoio oferecidos para a realização desta pesquisa.

Cellulose acetate composite membranes incorporating functionalized magnetic nanoparticles for oil/water emulsion separation

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Palavras Chave:*cellulose acetate,nanocrystal,iron oxide,wastewater,functionalization*

Highlights

Functionalized nanoparticles compatibility within polymer
Nanoparticle loading improved oil rejection
Composite membranes for efficient oil/water separation

Resumo/Abstract

Polymeric membranes based on cellulose acetate (CA) have been extensively investigated for oil/water emulsion separation; however, their practical application is often limited by insufficient selectivity and operational stability. In this study, commercial microcellulose was employed as a precursor for the synthesis of cellulose acetate via homogeneous acetylation, followed by the preparation of composite membranes incorporating oleic-acid-functionalized iron oxide (Fe_3O_4) magnetic nanoparticles to enhance separation performance. The $Fe(acac)_3$ precursor was synthesized and confirmed by Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). Solvothermal route yielded oleic-acid-functionalized Fe_3O_4 nanoparticles with a cubic inverse spinel structure. Nanoparticles and the resulting composite membranes were characterized by XRD, FTIR, and scanning electron microscopy (SEM). SEM analyses confirmed the successful incorporation of the nanoparticles into the CA matrix, revealing good dispersion and interfacial compatibility. Membrane performance was preliminarily evaluated through vacuum-assisted filtration of oil/water emulsions, analyzing permeate flux and separation efficiency by UV–Vis spectrophotometry. The results demonstrated that increasing the magnetic nanoparticle content (1, 3, and 5 wt%) led to a progressive improvement in membrane performance, characterized by enhanced oil retention selectivity while maintaining adequate permeation fluxes. Overall, the structural, morphological, and filtration results indicate that oleic-acid-functionalized magnetic nanoparticles act as effective functional additives in CA-based membranes, highlighting their potential for application in oily wastewater treatment.

Agradecimentos/Acknowledgments

The authors acknowledge CAPES, CNPq, FAPES, and UFES for financial and structural support.

Cellulose and PVA-based aerogels from the DMSO/DBU/CO2 system

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Palavras Chave:*regenerated cellulose, polyvinyl alcohol, CO2-switchable solvent, composite aerogels;*

Highlights

The objective of this work was to obtain composite aerogels based on regenerated cellulose and polyvinyl alcohol, using the DMSO/DBU/CO_2 system as the dissolution medium.

Resumo/Abstract

Several studies in the literature have reported the successful preparation of aerogels, hydrogels, and cryogels using cellulose and PVA as main components. Among the solvent systems used for the production of some of these materials are NaOH/urea and LiCl/DMAc, in addition to the use of ionic liquids, such as 1-butyl-3-methylimidazolium chloride. However, in none of these cases was the DMSO/DBU/CO_2 system used. This solvent system allows cellulose to be dissolved from the formation of cellulose carbonate, a species soluble in DMSO. In addition, DMSO has a high solubilization capacity for PVA, a factor that contributes to obtaining a homogeneous solution for the production of materials. Thus, in addition to allowing the components to be dissolved quickly and at a mild temperature, the DMSO/DBU/CO_2 system is low cost and easy to recycle. Thus, for the preparation of cellulose and PVA-based aerogels, the DMSO/DBU/CO_2 system was used as the dissolution medium, followed by the addition of antisolvents to promote the physical crosslinking of materials. Subsequently, the systems were subjected to the freeze-drying process to obtain the aerogels. The main objective of this study was to explore the properties of the prepared materials, as well as to evaluate the influence of varying proportions between the components on the final properties. Figure 1 shows the SEM of the fracture of the aerogel consisting of 50/50 cellulose and PVA, in which a porous structure with cross-links is observed, with no evidence of phase separation between the two components.

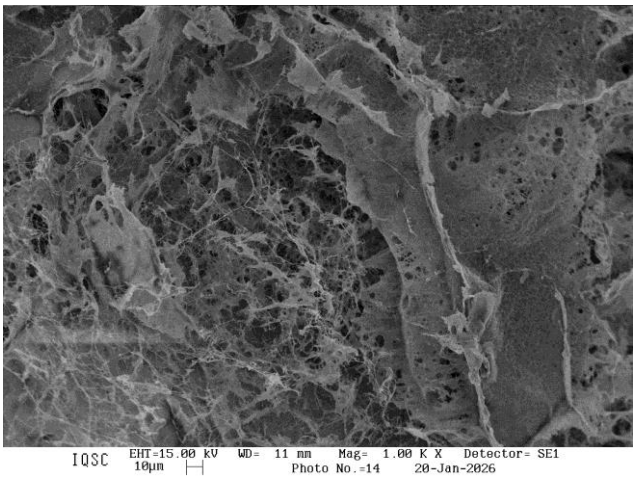


Figure 1: SEM image of the fracture of the aerogel obtained, composed of 50/50 cellulose and PVA.

Agradecimentos/Acknowledgments

To FAPESP (2025/05651-7) for funding the project.

Cellulose–Carbon Black Cryogels as Functional Materials Combining Mechanical Performance and Antistatic Properties

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Palavras Chave:*antistatic packaging, cryogels, microfibrillated cellulose, carboxymethylcellulose, carbon black*

Highlights

Conductive and mechanically robust cryogels were obtained from cellulosic materials and carbon black, exhibiting composition-dependent properties, aimed at antistatic packaging applications.

Resumo/Abstract

In the electronics industry, antistatic packaging is essential to prevent damage caused by electrostatic discharge during the storage and transportation of electronic components. To perform this function, materials must exhibit low electrical resistance and dissipative properties capable of conducting electrons through their structure. Most available solutions are based on polymers derived from non-renewable sources, whose slow degradation leads to significant environmental impacts. In this context, this work proposes the development of conductive cryogels based on microfibrillated cellulose (MFC), carboxymethylcellulose (CMC), and carbon black (CB), targeting their application in more sustainable antistatic packaging. In addition to being renewable and biodegradable, the cellulose-based materials used are commercially available, and no chemical modifications were required, increasing the applicability and potential scalability of the process. The formulations varied only in the MFC/CMC ratio, while the CB content was kept constant. Physical and mechanical characterizations revealed low-density cryogels (45–55 mg cm^{-3}) with high porosity (94.8–95.8%), typical of lightweight cellulosic materials, along with good mechanical performance, achieving a specific modulus of up to 76 $MPa \cdot cm^3 \cdot g^{-1}$ at low relative humidity (21% RH). Under these conditions, some formulations exhibited electrical conductivity, which depended on the CMC/MFC ratio. When exposed to high relative humidity (85% RH), the cryogels showed significant changes in their electrical and mechanical properties, attributed to the strong interaction of water with the polysaccharide matrix, which enhances ionic mobility and exerts a plasticizing effect. Overall, the results demonstrate that cellulose-based cryogels combined with carbon black offer a promising balance between mechanical performance and tunable electrical conductivity, reinforcing their potential as antistatic materials for packaging applications.

Agradecimentos/Acknowledgments

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Chemical modification of Amazonian fibers for the production of fluorescent sensors aimed at removing and detecting toluene from the atmosphere.

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Palavras Chave:*Amazonian adsorbents,Agro-industrial waste,Organic contaminants*

Highlights

Novel hybrid adsorbent developed from Amazonian Babaçu fibers.

Rapid kinetics resulted in >95% toluene removal in 12 hours.

Fluorescent fibers effectively detect toluene via quenching.

Resumo/Abstract

Atmospheric contamination by organic compounds poses significant environmental and public health risks [1]. Among remediation techniques, adsorption coupled with detection stands out for its simplicity and economic viability [2]. This study develops fluorescent adsorbents by chemically modifying Amazonian Babassu fibers with Carbon Quantum Dots (CQDs) for the efficient removal and detection of atmospheric toluene. CQDs were synthesized via a hydrothermal method using propylene glycol and grafted onto the fibers through citric acid polycondensation, using KH_2PO_4 as a catalyst. Characterization confirmed the effective incorporation of CQDs on the fiber surface. Morphological analyses (SEM/TEM) revealed altered surface roughness, while FTIR confirmed the presence of specific carboxylic and nitrogenous functional groups. Additionally, N_2 adsorption/desorption assays demonstrated a significant increase in the adsorbent's surface area compared to the raw material. Remediation performance, evaluated in a closed volatilization system, indicated a fast-kinetic interaction, achieving toluene removal rates exceeding 95% in 0,5 h —a notable contrast to the unmodified fiber, which showed negligible adsorptive potential. Finally, fluorescence spectroscopy validated the material's dual functionality: the fibers act as optical sensors, detecting toluene through a fluorescence quenching mechanism, even in environments containing interferents. This approach successfully valorizes agro-industrial waste for sustainable environmental applications.
Reference:
[1]LI, Rong et al. Health risk assessment of volatile organic compounds (VOCs) emitted from landfill working surface via dispersion simulation enhanced by probability analysis.*Environmental Pollution*, v. 316, p. 120535, 2023. https://doi.org/10.1016/j.envpol.2022.120535
[2]SOPHIA, C. A.*et al.*Removal of emerging contaminants by adsorption.*Ecotoxicol Environ Saf.*, 2018. https://doi.org/10.1016/j.ecoenv.2017.12.026

Agradecimentos/Acknowledgments

The authors thank CMABio-UEA for microscopy, Electrochemistry Lab-UFAM for facilities, and CAPES and CNPq for financial support.

Chemical vapor deposition growth of 2D High Entropy Transition Metal Dicalchogenides: characterization and systematic evaluation of reproducibility

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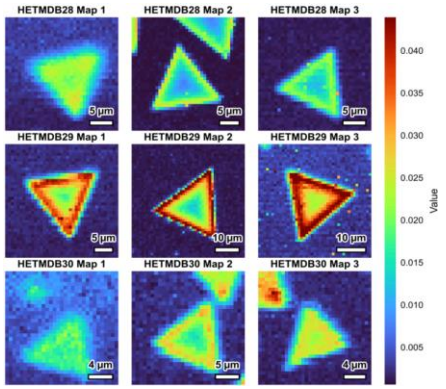
Palavras Chave:*High-entropy materials, Transition metal dichalcogenides, Chemical vapor decomposition, Reproducibility, Systematic evaluation,High-entropy materials,,High-entropy materials,Transition metal dichalcogenides,Chemical Vapor Deposition,Reproducibility,Systematic evaluation*

Highlights

High-entropy alloying enables spatially uniform defect engineering in CVD-grown TMDs. Statistical spectroscopy and microscopy confirms high intra-sample homogeneity and batch-to-batch reproducibility.

Resumo/Abstract

The growing demand for advanced materials for renewable energy applications has intensified the interest in transition metal dichalcogenides (TMDs). Defect engineering has emerged as an effective strategy to tailor their physicochemical properties. However, most reported approaches rely on localized functionalization. Here, we propose a high-entropy (HE) alloying strategy to induce defects in a spatially uniform manner in MoS_2 monolayers (ML) synthesized by chemical vapor deposition (CVD). The synthesis was performed using S_8 and a mixture of Mo with W, V, Nb, and Ta oxides with NaCl as a growth promoter. After synthesis, optical microscopy, non-resonant Raman (NRR), resonant Raman, and photoluminescence (PL) measurements were systematically conducted to assess homogeneity and reproducibility. Three samples were produced in sequential batches, each subdivided into 9 regions to ensure statistically representative datasets. Statistical analysis combining all spectroscopic data revealed high intra-sample homogeneity, while minor statistical differences were observed between batches. Spearman correlation coefficients above 95% were obtained for the average NRR spectra among samples, whereas PL showed greater sensitivity to subtle variations in defect distribution. Statistical evaluation of optical microscopy images revealed a significantly variation of layers thickness distribution, while the flakes' lateral size and total substrate coverage remains statistically similar across samples. The samples presented an average ML coverage of 12.10 ± 2.87% and an average flake size of 20.44 ± 3.52 μm, indicating a robust and homogeneous growth process. NRR spectra revealed contributions from both 2H and 1T′ phases, as well as defect-related modes, confirming effective defect engineering through the HE alloying approach. Overall, this methodology provides a systematic and statistically grounded framework for reproducible synthesis of HETMD MLs by CVD.



Raman mapping of 3 flakes of each sample - LA(M) vibrational mode (230 cm-1), normalized intensity.

Agradecimentos/Acknowledgments

We acknowledge financial and institutional support from CNPq, CAPES, PGQu, INCT, Serrapilheira and FAPERJ, as well as infrastructure from LARHCO and PUC-Rio, and valuable discussions with Dr. Alex S. Lima.

Chirality Induction in MoS2 Nanostructures for the Development of Hybrid Systems with Plasmonic Nanoparticles

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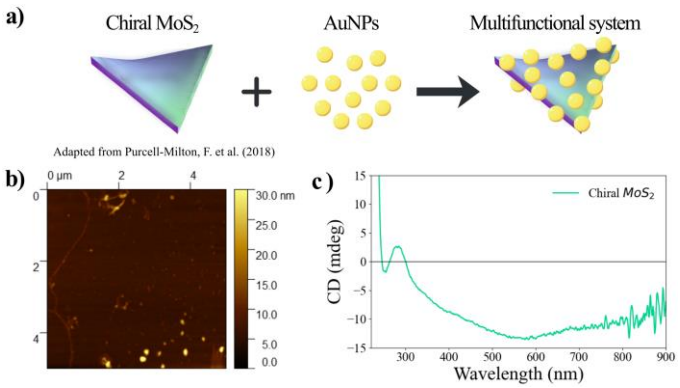
Palavras Chave:*Bidimensional Materials,Molybdenum Disulfide,Chiral Nanostructures,Plasmonic Nanoparticles*

Highlights

Few-layer MoS2 nanosheets obtained by controlled liquid exfoliation under N2 atmosphere, L-cysteine-induced chiral functionalization as evidenced by Circular Dichroism spectroscopy.

Resumo/Abstract

Transition metal dichalcogenides are promising bidimensional materials due to their high surface area and structure-dependent properties. The introduction of chirality into 2D systems is an emerging strategy to expand their optical and chemical functionalities, although chiral hybrid nanostructures remain largely unexplored. Thus, this work focuses on the development of chiral MoS2 nanosheets as a platform for in situ growth of plasmonic gold nanoparticles (AuNPs), aiming to investigate the influence of chirality on nanoparticle formation. MoS2 monolayers were obtained through a top-down method based on liquid exfoliation in isopropanol (IPA) under ultrasonic bath and a nitrogen (N2) atmosphere, followed by an exfoliation step in degassed water. Chirality was induced utilizing the chiral amino acid L-cysteine using ultrasound and under N2 in an aqueous medium. Several parameters for exfoliation and functionalization were evaluated to minimize oxidation and improve MoS2 stability. UV-Vis spectra showed the four characteristic peaks of excitons from exfoliated MoS2 and AFM revealed flakes with a lateral size of about 140 nm and heights varying from 1 to 5 nm. Raman revealed the main modes for the semiconductor phase of 2H-MoS2 and Circular Dichroism (CD) spectroscopy indicates a successful induction of chirality after functionalization with L-cysteine. As a perspective, in the short term, the focus will be on optimizing the functionalization and chirality induction steps to improve stability and chiral behavior. In the long term, the goal is to use this chiral MoS2 platform for the in situ growth of AuNPs. This hybrid platform can exhibit multifunctional and synergistic properties that may be attractive for applications ranging from energy to medical devices.



a) Diagram of the hybrid platform; b) AFM image of exfoliated MoS2; c) CD spectrum of chiral MoS2.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP through the fellowship (No.2025/11877-8) and CEPID CEMol (No. 2024/00989-7), as well as research support from LNNano/CNPEM for Raman measurements and LNBio/CNPEM for Circular Dichroism facilities.

Chitosan Functionalized with 4-Formylphenylboronic Acid for Targeted Phytosome-Based Polyphenol Delivery

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Palavras Chave:*chitosan,4-formylphenylboronic acid,phytosomes,polymer,nanotechnology*

Highlights

Chitosan functionalization enabling co-delivery of quercetin and resveratrol in phytosomal nanocarriers. Boronic acid–mediated interactions as a strategy for targeted polyphenol delivery.

Resumo/Abstract

This work aims at the functionalization of a biopolymer for the targeted coating of nanocarriers. To overcome the low bioavailability of polyphenols with antiallergic potential (quercetin and resveratrol), chitosan (CS), a biocompatible polymer, was functionalized with 4-formylphenylboronic acid (FPBA) groups through reductive alkylation using sodium borohydride, resulting in the attachment of FPBA moieties to the polymer chain. The central hypothesis is that FPBA modification will confer both colloidal control and active targeting capability to CS when used as a phytosome coating material, taking advantage of the specific affinity of boronic acid for sialic acid molecules, which are overexpressed at inflammatory sites. The synthesized CS-FPBA polymer was characterized by ^{1}H-NMR, confirming a degree of substitution of 13%. Its performance as a coating material was evaluated in polyphenol-loaded phytosomes. The results showed that CS-FPBA coating modifies the surface properties of phytosomes, inverting the zeta potential from −20 mV to +23 mV and reducing the average particle size from ~900 nm to ~760 nm, indicating successful electrostatic deposition and colloidal stabilization. In addition, CS-FPBA coating altered the release kinetics, inducing a sustained release profile compared with uncoated phytosomes. These findings demonstrate that FPBA functionalization is an effective strategy to transform chitosan into an active coating material capable of modulating surface charge and release dynamics. This material platform shows strong potential for the rational design of targeted delivery systems in biomedical applications.

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Number 2025/21209-2. We acknowledge the School of Pharmaceutical Sciences of Ribeirao Preto for institutional support.

Close-Packed Gold and Silver Nanocube Assemblies Enabling Highly Sensitive SERS Detection of L-Dopa

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Palavras Chave:*Surface-Enhanced Raman Scattering (SERS),Gold and Silver Nanocubes,Plasmonic Nanostructures,Levodopa Detection,Self-assembly Nanostructures*

Highlights

Close-packed Au and Ag nanocube assemblies were developed as efficient plasmonic SERS substrates. The SERS platforms enabled sensitive and reproducible detection of L-Dopa from 10^{-3} to 10^{-10} mol L^{-1}.

Resumo/Abstract

Parkinson's disease is a neurodegenerative disorder of the central nervous system associated with the progressive loss of dopaminergic neurons, resulting in dopamine deficiency. Levodopa (3,4-dihydroxyphenylamine, L-Dopa) is a catecholamine-based drug widely used to restore dopamine levels in the brain, making its fast and accurate detection highly relevant. Raman spectroscopy is an efficient analytical technique for molecular identification; however, its application to catecholamine compounds is limited by strong fluorescence backgrounds and intrinsically weak Raman scattering, particularly at low concentrations. These limitations can be overcome by surface-enhanced Raman scattering (SERS), which exploits plasmonic metallic nanostructures to amplify Raman signals. Gold and silver nanocubes (AuNCs and AgNCs) are especially attractive SERS substrates due to their sharp edges and corners, which create intense electromagnetic hot spots and additional plasmonic modes, thereby enhancing analytical sensitivity. In this work, we evaluated the performance of SERS substrates based on close-packed assemblies of AuNCs and AgNCs for the detection of L-Dopa over a concentration range from 10^{-3} to 10^{-10} mol L^{-1}. AuNCs coated with a hexadecyltrimethylammonium bromide (CTAB) bilayer exhibited a positive surface charge, while AgNCs stabilized with polyvinylpyrrolidone (PVP) showed a slightly negative surface charge. Scanning transmission electron microscopy (STEM) revealed narrow size distributions, with average sizes of 55.3 ± 4.6 nm for AuNCs and 57.8 ± 5.1 nm for AgNCs. UV-Vis spectroscopy showed localized surface plasmon resonance bands at 532 nm for AuNCs and 476 nm for AgNCs. The developed SERS substrates demonstrated high sensitivity and good reproducibility for L-Dopa detection across the entire investigated concentration range, with AuNC-based substrates showing superior selectivity compared to AgNCs.

Agradecimentos/Acknowledgments

FAPESP (2022/02893-1), INCT/INOMAT, UNICAMP-IQ, Laboratório Multiusuário de Espectroscopia Óptica Avançada (LMEOA), LNNano, CNPq, Capes.

Cobalt- and Copper-Modified NiFe Layered Double Hydroxides for Catalytic Reduction of 4-Nitrophenol

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Palavras Chave:*Wastewater; Nitrobenzene Compounds; LDH; 4-nitrophenol; Catalytic Reduction*

Highlights

NiFe-based LDHs containing cobalt and copper were synthesized.

The materials were applied in the catalytic reduction of 4-nitrophenol.

Copper-based LDHs showed superior kinetic performance.

Resumo/Abstract

The presence of toxic organic compounds in wastewater is one of the most challenging environmental pollution problems, among which nitrobenzene compounds stand out, especially 4-nitrophenol[1]. Therefore, new techniques for the removal of these pollutants have been proposed due to the low efficiency of conventional processes. A widely used approach is the catalytic reduction of these compounds to anilines, which are less toxic and employed in industry, particularly in the pharmaceutical sector. However, these catalysts are generally based on noble metals, making the development of catalysts based on more abundant metals of great interest. Among these materials, layered double hydroxides (LDHs) have shown great potential and have been widely studied. These materials consist of layers containing two metallic cations and intercalated hydrated anions2. Thus, NiFe LDHs with different cobalt contents, denoted as NiFeCo0.5, NiFeCo1, and NiFeCo2, as well as NiFe LDHs with different copper contents, denoted as NiFeCu0.5, NiFeCu1, and NiFeCu2, were synthesized using a hydrothermal methodology3. The materials were applied in the reduction of 4-nitrophenol to 4-aminophenol using sodium borohydride as the reducing agent. Kinetic studies demonstrated that the copper-based catalyst exhibited a higher reaction rate than the cobalt-containing material, with a kinetic constant approximately 21 times higher (k_{app} = 22.15 min^{-1} for $NiFeCu_2$ and k_{app} = 1.06 min^{-1} for $NiFeCo_2$). The materials obtained exhibited magnetic properties, facilitating their separation and reuse. The results show that incorporating copper into NiFe LDHs increased catalytic efficiency compared to cobalt, highlighting NiFe LDHs based on Cu as promising materials for the reduction of nitroaromatic compounds in aqueous media.

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Agradecimentos/Acknowledgments

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Compositional Tuning of Cu2AgBiI6 Thin Film Solar Absorber via Alkali Metal Substitution: Synthesis and Characterization

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Palavras Chave:*Solar Cells,Perovskite,Lead Free*

Highlights

Lead-free Cu_2AgBiI_6 has good characteristics for photovoltaics, but it suffers from defect-mediated recombination. Alkali cation substitution is proposed to tune its properties, increasing efficiency.

Resumo/Abstract

Lead halide perovskite solar cells have achieved efficiencies above 25%, but the toxicity and instability associated with lead motivate the search for non-toxic alternatives. The quaternary halide Cu_2AgBiI_6 (CABI) is a recently identified, stable, all-inorganic semiconductor with a wide direct bandgap (~2.06 eV) and very high absorption coefficient (~10^5 cm^{-1}). These attributes make CABI attractive for tandem and indoor photovoltaics, yet unmodified CABI films suffer from defect-mediated recombination and poor device efficiency (~1–2%). Previous compositional tuning (e.g., mixed halides or Sb alloying) has been shown to reduce trap densities and improve carrier lifetimes, suggesting that alternative substitutions could further enhance performance.

In this project we will explore partial substitution of alkali-metal cations (Cs^+, Rb^+, K^+) into CABI thin films. We will prepare spin-coated films from iodide precursors (CuI, AgI, BiI_3) with controlled additions of CsI, RbI, or KI. Structural and morphological characterization will be performed by X-ray diffraction (XRD) and electron microscopy (SEM), while optical and electronic properties will be probed by UV–Vis absorption, photoluminescence (PL) and X-ray photoelectron spectroscopy (XPS). Advanced synchrotron-based measurements (X-ray microscopy and high-resolution XRD) will complement these techniques to link compositional changes with microstructure. Finally, device measurements will ensure what is observed in previous characterization.

We hypothesize that the alkali ions will change and passivate defect sites, potentially inducing a band-gap shift. Such tuning is expected to extend charge-carrier lifetimes and enhance power-conversion efficiency in CABI devices. By establishing composition–structure–property relationships for alkali-doped CABI, this work aims to advance the design of efficient lead-free, thin-film solar absorbers.

Agradecimentos/Acknowledgments

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Construction waste residues as precursors for cementitious and geopolymeric materials: a valorization approach

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Palavras Chave:*Construction waste, Cementitious materials, Geopolymers, Physicochemical characterization, Circular economy*

Highlights

Construction waste residues evaluated as precursors for advanced materials
Physicochemical characterization guiding cementitious and geopolymeric routes

Resumo/Abstract

The reuse of construction and demolition waste represents a strategic challenge for sustainable development and the implementation of circular economy practices, particularly in the context of public works. In this study, the potential of construction waste residues as precursors for the development of cementitious and geopolymeric materials is evaluated, with emphasis on their physicochemical properties and mechanical performance.

Residue samples were collected from different types of public construction sites, including renovation, demolition, and earthworks, and were subjected to preliminary classification and particle size analysis. Physicochemical characterization was carried out using techniques such as X-ray diffraction (XRD), X-ray fluorescence (XRF), infrared spectroscopy (FTIR), and particle size distribution analysis, enabling the identification of mineralogical composition, oxide content, and material reactivity.

Based on the obtained results, selected residues were evaluated as partial substitutes in cementitious formulations and as precursors in geopolymeric systems. Mechanical performance was investigated through compressive strength tests at different curing times, allowing comparison among different residues and formulation strategies. The tests indicated that certain residues exhibit suitable properties for the formation of cementitious and geopolymeric matrices, with competitive mechanical performance and potential to reduce the consumption of conventional raw materials.

In an integrated manner, the results indicate that residue composition and mineralogy play a decisive role in the formation and performance of cementitious and geopolymeric matrices, consolidating their use as precursors in sustainable materials development routes.

Agradecimentos/Acknowledgments

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Conversão de resíduos agroindustriais em nanomateriais funcionais: Carbon dots (CDs) a partir do bagaço de malte

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Palavras Chave:*Carbon dots,nanopartícula,bagaço de malte,resíduos*

Highlights

Sustainable synthesis of fluorescent carbon dots from brewery waste using a simple calcination–oxidation route.

Resumo/Abstract

Os Carbon dots (CDs) são uma classe de nanomateriais à base de carbono com crescente interesse científico devido às suas propriedades de fluorescência, estabilidade química, biocompatibilidade e ampla aplicação em diversas áreas como biotecnologia, farmacologia e remediação ambiental. Esses nanomateriais podem ser obtidos a partir de diferentes fontes de carbono, como moléculas orgânicas sintéticas, biomassa e resíduos agroindustriais, destacando o caráter sustentável dessa classe de materiais e sua alinhamento com os ODS da ONU. Nesse contexto, o bagaço de malte, resíduo gerado em abundância pela indústria cervejeira, apresenta alto teor de matéria orgânica, alta perecibilidade e baixo valor agregado, configurando-se como um precursor promissor para a síntese de nanomateriais de alto valor tecnológico, contribuindo especialmente para os ODS 9 e 12. Diante disso, foi realizada a síntese de CDs a partir do bagaço de malte por meio da calcinação seguido por oxidação química. As nanopartículas obtidas foram caracterizadas pelas técnicas de espectroscopia de UV-vis, fluorescência e FT-IT. As caracterizações indicaram banda de absorção em 300 nm, atribuída às transições eletrônicas do tipo $n \rightarrow \pi^*$, característica de compostos carbonílicos presentes na superfície das nanopartículas. De forma complementar, observou-se emissão fluorescente dependente do comprimento de onda de excitação, com emissão máxima em 440 nm quando excitadas em 340 nm, cujo comportamento é típico dos múltiplos centros emissores da superfície dos CDs. Além disso, as nanopartículas apresentaram superfície altamente funcionalizada, contendo grupos como hidroxila, carbonila e metila, os quais contribuem para a solubilidade em meio aquoso e estabilidade coloidal. Em conjunto, os resultados evidenciam a viabilidade da conversão de resíduos agroindustriais em nanomateriais funcionais, reforçando o papel da nanotecnologia no desenvolvimento de soluções inovadores e sustentáveis.

Correlation between hydrothermal synthesis conditions and structural properties of Nb2O5 nanostructures.

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Palavras Chave:*Niobium pentoxide, Catalytic materials, Hydrothermal synthesis,Niobium pentoxide,Catalytic materials,Hydrothermal synthesis*

Highlights

A tenfold increase in reagent concentration results inno significant structural changes in Nb_2O_5 synthesized hydrothermally at 120–150°C, without compromising its structural properties.

Resumo/Abstract

Niobium oxides exhibit promising catalytic properties in the production of biofuels, the generation of green hydrogen, and other applications. Niobium pentoxide (Nb_2O_5) stands out as a catalyst due to its high surface area, the presence of Brønsted and Lewis acid sites, and its high thermal stability. Although the hydrothermal synthesis of Nb_2O_5 is widely reported in the literature, this method typically yields a low molar yield (close to 15%). In order to increase the amount of Nb_2O_5 produced, this work proposes multiplying the concentration of the reagents by 10 times, under temperatures of 120 and 150 °C, in order to evaluate the effects of these conditions on the structural properties of the material obtained. In this work, hydrothermal synthesis was employed using ammonium niobium oxalate and hydrogen peroxide, in the Nb^{5+}:H_2O_2 molar ratio of 10:1. The concentration of the reagents was increased by a factor of 10, while maintaining the ratio and volume between them.

Using Raman spectroscopy and X-ray diffraction (XRD) techniques, it was possible to verify that no significant structural changes occurred as a function of the variation in reagent concentration during synthesis. The XRD diffractograms indicate similar phases with a predominance of the amorphous phase, with growth preference in the (001) direction, characteristic of nanorod-type morphology, corroborated by transmission electron microscopy images. Consistently, the Raman spectra do not reveal significant differences in the degree of structural disorder, the presence of defects, or the characteristics of the crystal lattice between the different synthesis conditions.

Therefore, with the results obtained, it is possible to conclude that increasing the concentration of reagents by 10 times at different temperatures of 120 and 150ºC does not significantly alter the structural properties of the catalysts, in equal synthesis volumes.

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CO2 capture and conversion in Ca-modified biochars: effects of temperature and humidity.

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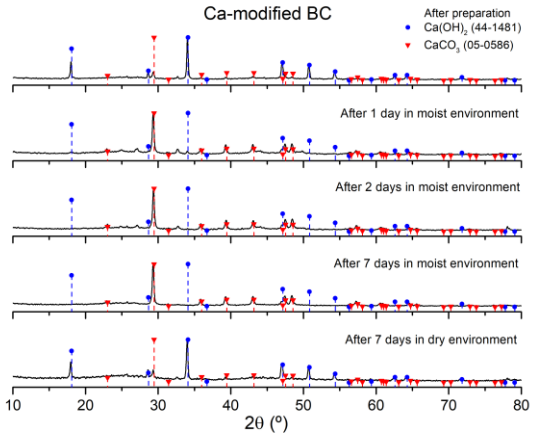
Palavras Chave:*Biochar, CO2 adsorption, CO2 conversion, carbonation, humidity.*

Highlights

Ca-modified biochars adsorb and store CO_2. Carbonation occurs at room temperature under humid conditions. Moisture in the porous carbon promotes carbonation.

Resumo/Abstract

Carbon capture and storage (CCS) are technologies that enable the reduction of atmospheric CO_2 levels, contributing to the mitigation of the impacts of global warming and climate change. Several adsorbents are employed for CO_2 capture, such as biochar (BC), which is a low-cost and widely available material. Despite this, few studies have been reported dealing with CO_2 capture followed by storage using BCs. This work presents an investigation about the adsorption, conversion, and storage capacity of CO_2 in porous BC samples containing calcium (Ca), derived from a biomass precursor, evaluating their performance under different temperature and humidity conditions. The results obtained showed that Ca-modified BCs are capable of adsorbing and storing CO_2 in the form of carbonates, both at high temperatures and, when under humid ambient conditions, even at room temperature. Thermal treatment at 510 °C indicated that the carbonation of the samples was favored by the increase in $Ca(OH)_2$ content (6.3 – 43.8 wt. %), leading to the formation of $CaCO_3$. In addition, the carbonation of the BC samples at room temperature was influenced by humidity, as the X-ray diffraction (XRD) patterns (Figure 1) showed that carbonation at room temperature occurred considerably faster in humid environments than in dry ones. The results of this study demonstrate that Ca-modified BCs are environmentally friendly hybrid adsorbents potentially useful for CCS, with the relatively large porosity and the hydrophilic character of the porous carbon matrix providing an environment rich in water that facilitates the carbonation process.



XRD patterns of Ca-modified BC before and after carbonation in dry and humid environments.

Agradecimentos/Acknowledgments

FAPES, CAPES, CNPq, UFES.

Cyclodextrin-based host-guest complexes with promising anti-Trypanosoma Cruzi activity: A solid-state formulation strategy for benznidazole.

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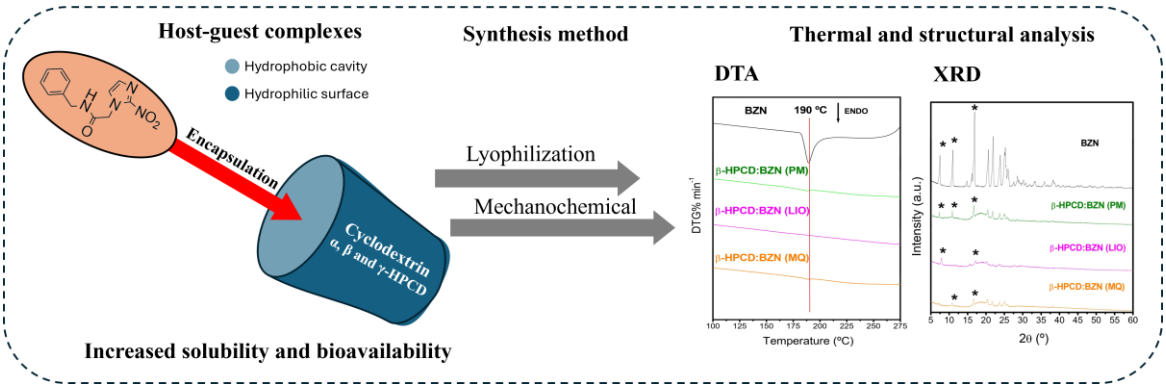
Palavras Chave:*Benznidazole,Chagas Disease,Cyclodextrins,Inclusion Complex,Drug Optimization*

Highlights

Cyclodextrin complexation aims to improve benznidazole solubility; CD torus size is a key parameter for complex formation; Hydroxypropylation of cyclodextrin is also key to obtain stable complexes.

Resumo/Abstract

This study addresses the key limitation of benznidazole (BZN), its low solubility which hinders its efficacy as the first-line treatment for Chagas disease. To overcome these challenges, solid-state inclusion complexes were developed with a series of cyclodextrins: α-cyclodextrin (αCD), β- cyclodextrin (βCD), and their hydroxypropylated derivatives (α-HPCD, β-HPCD, and γ-HPCD). To obtain the solid-state complexes, two methods were employed: the mechanochemical method, involving ball milling of the precursors for three hours; and the lyophilization method, based on the solubilization and stirring of the components in water for 72 hours, followed by freeze-drying. For comparative analysis, a physical mixture (PM) of the components was also prepared by grinding in an agate mortar. The characterization of the obtained systems was performed using ^{1}H-NMR, FTIR, DTA and XRD. Firstly investigations of in-solution interactions proceeded using ^{1}H-NMR, via dislocation of aromatic BZN Hs peaks. Such evidence was not obtained for α-cyclodextrins-BZN complexes, being confirmed by solid-state techniques, such as FTIR and DTA analyses which results reproduced those of PM sample. In contrast, significant 1H-NMR chemical shifts dislocations of the same BZN Hs were observed employing β-CD and hydroxypropylated derivatives (β-HPCD and γ-HPCD). The solid-state characterization of such samples evidenced disappearance of BZN melting point peak by DTA; and phase amorphozation by XRD, hence demonstrating the effectiveness of these preparation routes in stabilizing the host-guest complex. In conclusion, inclusion complexation optimized the properties of benznidazole. Both complex containig-β-HPCD and γ-HPCD emerged as the most promising systems by forming a stable complex, validated by both in-solution and solid state characterizations. These findings support HPCD use in drug development to overcome BZN's solubility/stability issues, enabling greater efficacy in Chagas disease therapy.



Schematic synthesis and thermal and structural analysis of inclusion complexes

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Data-Driven Optimization of Biochar production for High-Performance Supercapacitor Applications

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Palavras Chave:*energy storage, carbonaceous materials, biomass, data mining, machine leaning*

Highlights

Literature mining built a dataset on biochar use for supercapacitor electrodes. Production parameters influence the biochar properties. Deep learning is being used to optimize biochar properties.

Resumo/Abstract

The increase in energy demand resulting from population growth and technological development, has led to interest in new energy sources and storage devices. Supercapacitors appear to be a great alternative to energy storage devices due to their high power density and excellent cyclability. Among the different materials investigated for supercapacitor electrodes, biochar has attracted attention due to its low cost and renewable origin. Biochar presents high surface area and good electrical conductivity, and these properties depend on the production method (pyrolysis, hydrothermal carbonization, gasification), biomass precursor, temperature, and residence time. Additionally, the incorporation of nanoparticles and dopants can improve its specific capacitance. Therefore, there are several pathways to optimize synthesis parameters in order to achieve the best performance for supercapacitor electrode application. Due to it, this work aim to use machine learning techniques to predict biochar properties and correlate them with its productions parameters. Inicially, scientific abstracts were collected from Web of Science, and data (such as biomass precursor, production method, pre- and post-treatments, and electrochemical properties) was extracted using a python algorithm. The results revealed important trends, such as an increase in publications over time, and the predominance of agricultural waste as a biomass precursor. It was also observed that 43,2% of the abstracts reported some type of post-treatment. The density plots showed that most specific capacitance values were between 10 and 500 F g^{-1}, while the energy and power density distributions were concentrated in the ranges of 20 - 50 Wh kg^{-1} and 30 - 600 W kg^{-1}, respectively. Based on these findings, the current focus is on applying deep learning techniques to around 28.000 full-text articles in order to predict biochar properties and optimize its performance for supercapacitor applications.

Agradecimentos/Acknowledgments

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Desenvolvimento de um espectrômetro UV-VIS para a utilização em biossensores fotônicos.

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Palavras Chave:*Impressão 3D,biossensores fotônicos,espectrômetro Uv-Vis,instrumentação de baixo custo,DIY*

Highlights

Low-cost 3D-printed UV-Vis spectrometer for analytical applications.
Instrument tailored for photonic biosensor readout.

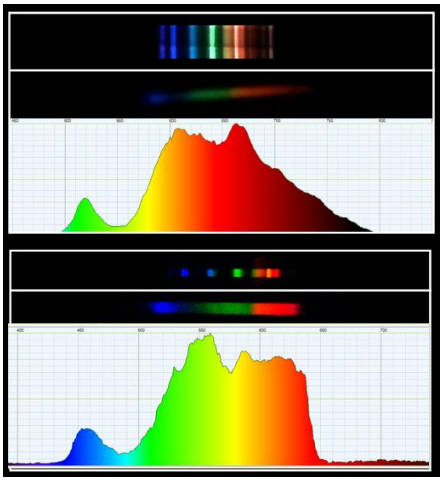
Resumo/Abstract

A crescente demanda por diagnósticos rápidos e acessíveis impulsiona o desenvolvimento de biossensores fotônicos para instrumentação analítica. Estes dispositivos exploram a interação entre biomoléculas e luz via estruturas plasmônicas, permitindo alta sensibilidade na detecção de patógenos. Nesse contexto, a impressão 3D surge como alternativa de baixo custo e flexibilidade funcional para a construção de sistemas de leitura espectroscópica.

Este trabalho tem com objetivo o desenvolvimento de um espectrômetro UV-Vis com estrutura impressa em 3D para leitura de biossensores fotônicos. O projeto foi modelado no software Tinkercad e impresso em filamento PLA preto. A captura espectral utilizou uma Arducam de 2 MP e uma webcam, com elementos dispersores de DVD ou grade de difração comercial de 1000 linhas/mm. Como fontes de luz, adotou-se um LED de 3 W e uma lâmpada halógena, com controle de intensidade via Arduino.

A seleção dos componentes considerou propriedades mecânicas, sensibilidade espectral e confiabilidade óptica. As geometrias foram inspiradas no espectrofotômetro NanoDrop® 2000, visando compacidade e análise de pequenos volumes; adicionalmente, desenvolveu-se também uma estrutura com caminho óptico expandido. A calibração inicial foi feita com lâmpada fluorescente, analisando as linhas de emissão de Hg, Eu e Tb. O processamento de imagens e espectros ocorreu nos softwares ImageJ, QtiPlot e Spectragryph.

As estruturas demonstraram capacidade de identificar variações no espectro visível na faixa de 200 a 800 nm, confirmando sua aplicabilidade analítica. Observaram-se flutuações de intensidade corrigidas por ajustes na potência dos emissores e no posicionamento da grade. As próximas etapas incluem a construção de curvas de calibração com corantes para determinar o limite de detecção e a faixa linear do equipamento.



Espectro de Absorção Uv-Vis de luz visível de ambas estruturas impressas.

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Desenvolvimento e caracterização de formulados de P123 para a incorporação simultânea de indirrubina e ftalocianina de alumínio-cloro

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Palavras Chave:*Terapia combinada, Sistemas nanoestruturados, Formulações, Fotossensibilizadores,Terapia Combinada,Indirrubina,Ftalocianina de alumínio-cloro,Plurônicos*

Highlights

• Dual encapsulation of AlPcCl and indirubin in Pluronic P123 micelles;

• Improved aqueous solubility and stability of the molecules;

• Combined photodynamic and bioactive therapeutic approach;

Resumo/Abstract

O câncer é uma doença preocupante, uma vez que dados internacionais preveem mais de 10,3 milhões de mortes por câncer neste ano. Terapias menos invasivas têm sido amplamente investigadas como alternativas aos tratamentos convencionais, como a quimioterapia e radioterapia. Nesse contexto, a terapia fotodinâmica (TFD) destaca-se por empregar fotossensibilizadores capazes de gerar espécies reativas de oxigênio sob irradiação luminosa. A ftalocianina de alumínio-cloro (AlPcCl) é um fotossensibilizador eficiente, entretanto, sua baixa solubilidade em meio aquoso e a tendência à agregação limitam sua aplicação direta, tornando necessário o uso de sistemas carreadores[1].

Além disso, a associação de compostos bioativos pode potencializar a eficácia terapêutica da TFD. A indirubina é um composto que apresenta propriedades anticancerígenas e atividade biológica independente da ativação luminosa[2]. Dessa forma, a combinação de um fotossensibilizador com um agente quimioterápico em um único sistema carreador pode resultar em efeitos terapêuticos sinérgicos.

Neste trabalho, foi desenvolvido um sistema micelar de Pluronic P123 para o encapsulamento simultâneo de AlPcCl e indirrubina (Figura 1), visando aumentar a solubilidade, a estabilidade e o potencial terapêutico do sistema. As formulações foram obtidas pelo método de dispersão sólida e caracterizadas por diferentes técnicas. O espectro de absorção UV-Vis da formulação (Figura 1) apresenta as bandas características da AlPcCl indicando a presença do fotossensibilizador predominantemente na forma monomérica. Além disso, a banda característica da indirrubina foi observada, confirmando sua incorporação no sistema micelar. As imagens de MET revelaram a presença de agregados circulares de diâmetro médio de 89,85 nm. Deste modo, os resultados até então obtidos indicam que o sistema desenvolvido promove a solubilização eficiente de ambos os compostos, mostrando-se promissor para aplicações em TFD associada a agentes bioativos.

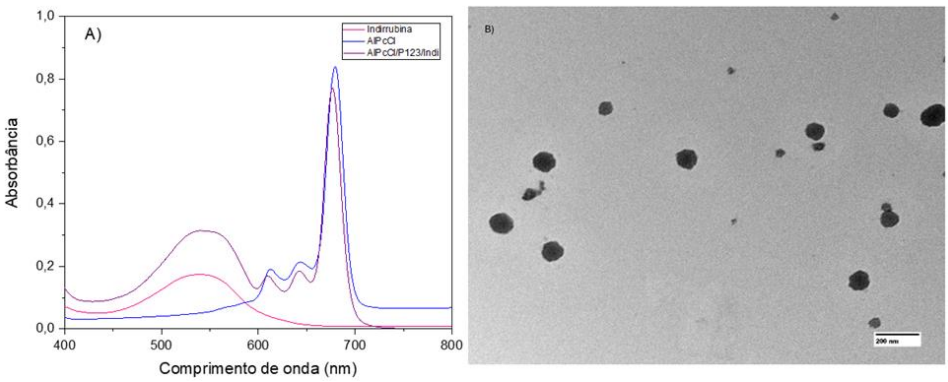


Figura 1. a) Espectro UV-Vis e b) imagem TEM do formulado.

Agradecimentos/Acknowledgments

Os autores agradecem ao CNPq – processos 302760/2025-3 e 441413/2023-4. Fundação de Apoio ao estado de Minas Gerais (FAPEMIG) – processo TEC BIS 00034/25

Development and characterization of nanoencapsulated systems containing magnetic nanoparticles applied to diagnostic imaging

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Palavras Chave:*Magnetic nanoparticles,Coating,Diagnosis,Imaging,Cancer*

Highlights

Zein-encapsulated magnetic nanoparticles DoE-optimized as a stable, low-toxicity contrast agent for cancer image diagnosis.

Resumo/Abstract

Nanotechnology has shown promising results in improving diagnostic accuracy and therapeutic efficiency, particularly in oncology, where targeted treatment and detailed visualization of affected tissue are essential. Nanoparticle coatings protect therapeutic agents from premature degradation, enable controlled release, enhance biocompatibility, reduce side effects and facilitate nanoparticles accumulation in target tissues. Among these systems, Magnetic nanoparticles, especially ferric oxide (Fe_2O_3), exhibit high potential for biomedical applications. This study proposes the development of zein-based nanoencapsulated systems containing citrate-stabilized ferric oxide magnetic nanoparticles for use as contrast agents in cancer imaging techniques, such as ultrasound and photoacoustic imaging. The methodology involves the synthesis of ferric oxide nanoparticles via the coprecipitation method, followed by sodium citrate functionalization and zein protein encapsulation. The resulting nanoparticles were characterized in terms of their magnetic, physical, and chemical properties. Citrate-coated magnetic nanoparticles exhibited an average diameter of 85,74 nm ± 2,39 nm, a Zeta potential of -33,43 mV ± 0,29 mV, and a polydispersity index (PDI) of 0,317 ± 0,024. Empty zein nanocapsules presented a diameter of 114,3 nm ± 12,2 nm, a Zeta potential of +12,57 mV ± 0,84 mV, and a PDI of 0,168 ± 0,046. Zein-encapsulated magnetic nanoparticles showed an average diameter of 121,87 nm ± 4,48 nm, a Zeta potential of +15,03 mV ± 0,67 mV, and a PDI of 0,156 ± 0,040. Additionally, parameters such as size, surface charge, polydispersity index, aggregation behavior, and release profile were analyzed using a Design of Experiment (DoE) approach to predict nanoparticle behavior under controlled experimental conditions, both with and without zein nanocapsules. This strategy enables the assessment of coating effects on contrast agent stability and imaging quality.

Agradecimentos/Acknowledgments

Authors thanks to the Unified Scholarship Program (PUB Project 3240/2025) from University of São Paulo.

Development of alginate and carrageenan biopolymer spheres for the creation of transdermal patches for THCA release.

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Palavras Chave:*THCA,Alginate,Carrageenan,Tetrahydrocannabinolic Acid*

Highlights

The research focuses on developing technologies for the efficient administration of Tetrahydrocannabinolic Acid (THCA), using biopolymers to create controlled-release systems.

Resumo/Abstract

Tetrahydrocannabinolic acid (THCA), a non-psychoactive component of cannabis sativa L., has promising therapeutic properties (anti-inflammatory, neuroprotective, antiemetic), without the psychoactive effects of tetrahydrocannabinol (THC). The use of biopolymers for the development of transdermal patches avoids first-pass metabolism by the liver, maintaining constant release levels (Pastore et al., 2015), in addition to proving to be an efficient and sustainable alternative.
This research aimed to develop and characterize colloidal spheres using biopolymers such as alginate and carrageenan as a matrix to microencapsulate THCA oil with the objective of creating controlled-release transdermal patches.
Three distinct samples were prepared in a 1 mol calcium chloride (CaCl2) solution, serving as a structuring and crosslinking agent, under magnetic stirring. In the first group, pure alginate spheres were dropped into the CaCl2 solution under stirring (translucent spheres). The second, alginate spheres with THCA (amber spheres). The third group, spheres of the polymer blend of alginate and carrageenan together with THCA (spheres slightly lighter than the second group and the solution somewhat cloudy), alginate and carrageenan are biocompatible, biodegradable and non-toxic biopolymers, all samples presented well-made spheres, subsequently stored in a falcon tube at 10oC. The material went on to characterization, where DSC, TGHA, FTIR-Raman and SEM analyses were performed. Considering the incorporation process, it is found that both the Alginate spheres and the Alginate and Carrageenan blend show promise for the creation of a potential transdermal adhesive for THCA release.

Agradecimentos/Acknowledgments

Acknowledgements: To CNPq, FAPEAL, and FINEP for their institutional and financial support.

Development of alginate-based hydrogels for the encapsulation and controlled release of fertilizers in agriculture.

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Palavras Chave:*Hydrogels,Nanocellulose,Controlled Release,Sustainable Materials,Fertilizers*

Highlights

Alginate-based hydrogels demonstrated potential for controlled nutrient release and reduced leaching losses in agricultural applications.

Resumo/Abstract

Conventional fertilization based on the use of traditional fertilizers (e.g., water soluble mineral fertilizers) is widely used in agriculture, though it is associated with environmental impacts arising from the uncontrolled release of nutrients, causing soil and water contamination. Hydrogels have been applied in agriculture due to their capacity to retain moisture and promote the gradual release of nutrients. Nevertheless, studies regarding the use of algae-based fertilizers for encapsulation and controlled release are still scarce. In this work, a sustainable alternative was developed to produce hydrogels for agricultural applications using marine algae fertilizers. Hydrogels were prepared by ionic gelification with calcium chloride and the incorporation of nanocelluloses, aiming to improve mechanical properties, stability, and functional performance. Release behavior was evaluated using methylene blue as a polar model compound, showing that the presence of CNC and CNF significantly altered the release profiles, resulting in faster release compared to the control alginate hydrogel, likely due to interactions between polar components and changes in pore structure. The practical performance of the encapsulated fertilizers was evaluated through a three-month romaine lettuce cultivation at Nord University, Norway, which showed higher soil electrical conductivity and increased leaf chlorophyll content for encapsulated systems, whereas soils treated with the non-encapsulated fertilizer retained higher carbon and nitrogen contents, indicating greater nutrient leaching. The results indicate that the developed hydrogels showed potential for agricultural applications, allowing greater control of nutrient availability, reducing losses by leaching, and mitigating environmental impacts. The ongoing study contributes to expanding knowledge on biomaterials based on algae biomass applied to sustainable agricultural development.

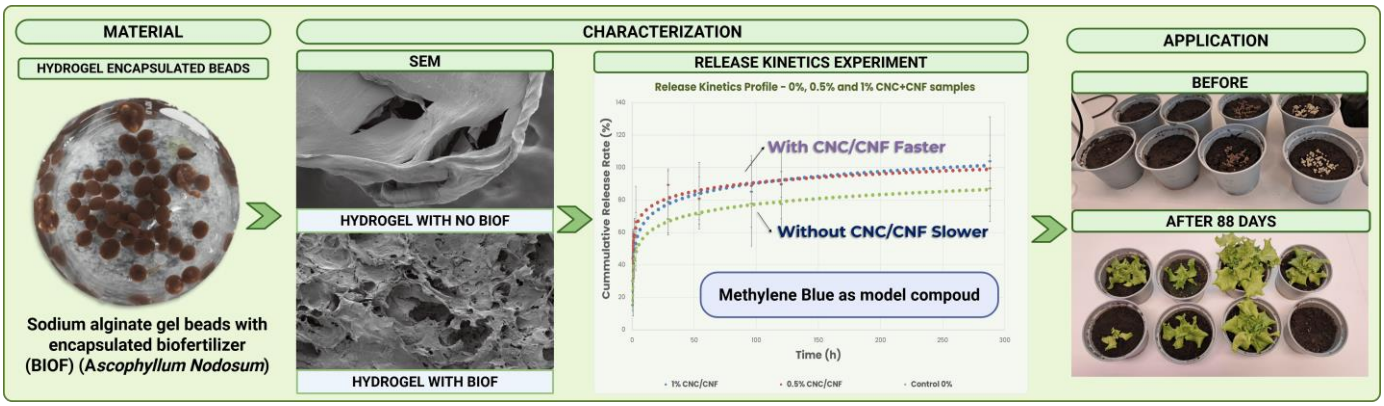


Figure. Alginate hydrogel beads with biofertilizer: SEM, release kinetics, and lettuce cultivation

Agradecimentos/Acknowledgments

The authors acknowledge CNPq, CAPES, Erasmus+, and Unicamp for financial support.

Development of a portable multifuncional reactor for adsorption reactions of potentially toxic metals in effluents using a composite Alg/MTT@CoFe2O4

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Palavras Chave:*Magnetic composite,Adsorption,Potentially toxic metals,Portable reactor*

Highlights

Portable reactor developed for in situ removal of toxic metalsAlg/MTT@CoFe2O4 composite ensures fast and efficient separationHigh adsorption capacity for toxic ions in a continuous flow system

Resumo/Abstract

The inadequate management of industrial waste has exacerbated the presence of potentially toxic metals in water bodies, necessitating the development of efficient and portable remediation technologies for in on-site applications. This work describes the development and validation of a portable fixed-bed reactor operating with a new magnetic composite adsorbent consisting of alginate, montmorillonite, and cobalt ferrite (Alg/MTT@CoFe,O4). The material was synthesized via chemical coprecipitation of nanoparticles followed by ionic gelation in the polymer matrix. Characterization by X-ray diffraction (XRD), vibrating sample magnetometry (VSM), and electron microscopy (SEM) confirmed the successful incorporation of the inorganic phase into the alginate network, resulting in spheres with a magnetic saturation of 42 emu g^{-1}, facilitating solid-liquid separation.
The reactor's performance was evaluated for the removal of Pb(II) and Hg(II) ions from synthetic effluents. In batch tests, the composite exhibited fast kinetics, reaching adsorption equilibrium in 40 minutes, with a mechanism governed by a pseudo-first-order model. The adsorption isotherms were best fitted by the Langmuir model, indicating monolayer deposition. In continuous flow mode within the prototyped reactor, operating at a flow rate of 10 mL min^{-1}, the system maintained a removal efficiency above 95% for treatment volumes of up to 200 bed volumes. The hydrodynamic and chemical stability of the spheres was confirmed after 8 consecutive adsorption-desorption cycles using an acidic solution (0.1 M HCl) as the eluent, with a capacity loss of less than 8%. The portable reactor demonstrated robustness and versatility, enabling decentralized effluent treatment. The Alg/MTT@$CoFe_2O_4$ system represents a viable, low-cost alternative for mitigating environmental impacts from heavy metals.

Agradecimentos/Acknowledgments

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Development of biomass-derived mesoporous carbon materials for CO2 capture.

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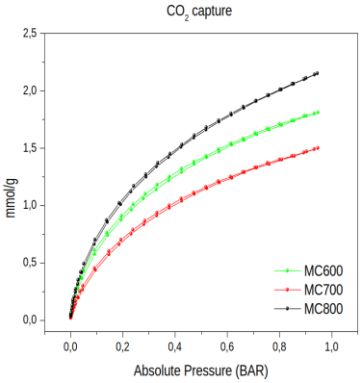
Palavras Chave:*Decarbonization,Adsorption,Nanomaterials,Biomass.*

Highlights

CO_2 capture using sustainable bio-based mesoporous carbons. Solvent-free synthesis from tannic acid creates a green, high-performance material for decarbonization.

Resumo/Abstract

In search of technologies capable of achieving atmospheric decarbonization, several alternatives have been developed. CO_2 capture proves to be a viable alternative for mitigating the intensification of the greenhouse effect. Various materials are studied for CO_2 capture. Among them, mesoporous carbon (MC) stands out due to their properties and the possibility of modifications that can enhance the capture efficiency of these materials. This work aims to study the synthesis of mesoporous carbons from biomass for CO_2 capture.
The synthesis of MCs was performed using the solvent-free method by mixing tannic acid (a biomass source), pluronic F127, and terephthalaldehyde (1:1:0,5 m/m) in a planetary ball mill, followed by pyrolysis at different final temperatures (600 °C, 700 °C, and 800 °C) to evaluate the effects of synthesis temperature on pore formation and its impact on CO_2 capture.
Thermogravimetric analyses showed that the three materials exhibited similar behaviors, with two-step degradation events. The first step involved a mass loss of approximately 5% at 100 °C, corresponding to the material's moisture content. A second stage degradation occurred between 350 and 520 °C, with a 90% mass loss attributed to carbon oxidation into CO_2. Nitrogen physisorption analysis revealed distinctions among the materials. MC800 exhibited the highest surface area at 557 m^2g^{-1}, while MC700 and MC600 showed more similar values, with areas of 483 and 498 m^2g^{-1}, respectively. This trend persists in pore size; MC700 and MC600 presented values of 6.48 and 6.50 nm, respectively, whereas MC800 displayed a smaller pore size of 5.60 nm. Finally, CO_2 capture tests demonstrated promising results, with MC800 yielding the highest capacity at 2.15 mmol g^{-1}, followed by MC600 at 1.81 mmol g^{-1}, and MC700 at 1.50 mmol g^{-1}.Although the work is still in progress, it already presents significant results, indicating a sustainable alternative for CO2 capture utilizing bio-based materials.



CO2 capture isotherms.

Agradecimentos/Acknowledgments

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Development of CMC and agroindustrial waste based composite inks for application in Direct Ink Writing 3D Printing

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Palavras Chave:*Direct Ink Writing,3D Printing,Carboxymethyl Cellulose,Agroindustrial Waste*

Highlights

Developed a low-cost, biodegradable composite ink focusing on waste material repurposing. Tests for DIW on an in-house modified 3D Printer. Validation of a printable prototype with banana peel filler.

Resumo/Abstract

In 2024, over 430 million tonnes of plastic were produced (Plastics Europe), of which only 9% is recycled and 19% incinerated (EEA), resulting in a large amount of plastic in landfills and in the environment. Concurrently, the agroindustrial sector generates a great amount of underutilised biomass: In Brazil alone, annual production includes 54.2 million coffee bags (CONAB), 7 million tonnes of bananas (IBGE), and over 57 billion eggs (ABPA). In that light, this work aims to develop a biodegradable and biocomposite ink using a carboxymethyl cellulose (CMC) matrix reinforced with organic filler, derived from agroindustrial waste. Ink compositions varying CMC, microcrystalline cellulose (MCC), glycerin, distilled water and processed banana peel biomass. This composition was used as filler in an ink for print tests. These were done on a commercial FDM 3D printer (Ender 3 V1) converted into a syringe extrusion based Direct Ink Writing (DIW) device. A slicing profile was created for the printer, the ink and for the prints on OrcaSlicer software. The criteria for the development of the ink are mainly its pseudoplastic properties, focusing on printability, digital model to artifact fidelity and the capacity for printing at least three stacked layers. The ink was validated through the printing of three-layer test structures. So far the main challenges have been the storage of elastic energy in the polymeric lattice structure, which provokes the unwanted and continued extrusion. The ink's rheology and the slicing profiles will be further improved aiming to fabricate of decorative artifacts. One possibility of such artifacts is the creation of biodegradable seedling pots which could be either printed or compression moulded, valuing technological mastery and offering a sustainable alternative to petroleum-based materials.



Picture of a multilayer test print of a CMC, MCC, glycerin, distilled water and banana biomass ink.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge the financial support of the CAPES. The authors also thank UFRJ, Labitan and Ladisp for providing the infrastructure and technical support necessary for this research.

Development of CuHCF@CNTf@FA@PVP Nanocomposites for Photodynamic Therapy in Cancer Treatment

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Palavras Chave:*Nanocomposites,Cancer treatmente,Photodynamic therapy*

Highlights

Cancer remains a leading cause of death, motivating nanocomposite-based strategies. CuHCF@CNTf@FA@PVP is proposed as a multifunctional platform with potential application in photodynamic therapy PDT.

Resumo/Abstract

Despite significant advances in cancer therapy, conventional treatments still suffer from limited specificity and dose-limiting toxicity, motivating the search for nanostructured systems capable of modulating therapeutic delivery at the nanoscale. In this context, nanocomposites are particularly attractive due to the synergistic integration of multiple components, enabling control over surface properties, colloidal stability, and functional performance. Hexacyanoferrate-based carbon nanostructures stand out as robust and versatile platforms for biomedical applications.

A copper hexacyanoferrate nanocomposite functionalized with carbon nanotubes and folic acid (CuHCF@CNTf@FA@PVP) was synthesized by a coprecipitation method. Potassium ferrocyanide, poly(vinylpyrrolidone), functionalized carbon nanotubes, and folic acid were simultaneously dispersed under magnetic stirring, followed by dropwise addition of copper nitrate to induce nucleation and growth. The suspension was stirred for 24 h, centrifuged, and washed to obtain the final material.

Raman spectra showed the D and G bands of carbon nanotubes at ~1340 and 1595 cm^{-1}, the 2D band, and the C≡N vibration around 2150 cm^{-1}. FTIR analysis confirmed C≡N (~2100 cm^{-1}), PVP bands at 1651 and 1350 cm^{-1}, and folic acid signals. Bands below 500 cm^{-1} in both techniques were attributed to metal–carbon interactions. XRD patterns revealed a cubic crystalline structure, while SEM images showed predominantly rounded cubic particles. UV–Vis spectra displayed absorption bands at ~300 and 550 nm.

Overall, the structural, morphological, and optical properties confirm the successful formation of a multifunctional nanocomposite with visible light absorption and biocompatibility, indicating its potential for photodynamic therapy applications. These combined features support its use as a light-responsive platform capable of efficient interaction with biological environments while preserving structural stability and versatility

Agradecimentos/Acknowledgments

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TeraNano.

Development of Nanoemulsions Containing Bimetallic Gold and Silver Nanoparticles (Au–Ag) for the Treatment of Cutaneous Leishmaniasis

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Palavras Chave:*Cutaneous leishmaniasis,Nanotechnology,Bimetallic nanoparticles,Gold and silver,Nanoemulsions*

Highlights

Development of bimetallic Ag@Au nanoparticles for cutaneous leishmaniasis;

Nanoemulsions for Ag@AuNPs dispersion and topical delivery;

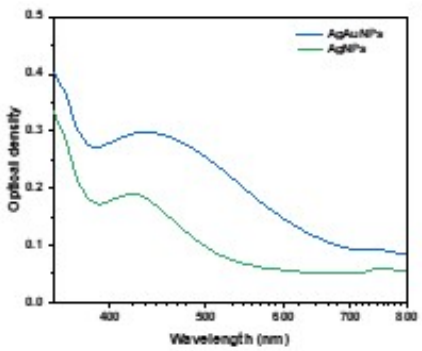
Enhanced antileishmanial activity from gold–silver synergism.

Resumo/Abstract

Neglected tropical diseases represent a major public health challenge, especially in developing countries, due to their high incidence, therapeutic limitations, and the scarcity of new treatment alternatives[1]. Among them, cutaneous leishmaniasis stands out for causing persistent ulcerative skin lesions and for relying mainly on systemic therapies associated with high toxicity, poor patient adherence, and the risk of parasite resistance[1]. In this context, nanotechnology emerges as a promising strategy for the development of safer topical systems[2]. This study proposes the development of oil-in-water nanoemulsions associated with bimetallic gold and silver nanoparticles (Ag@AuNPs), aiming at topical application for the treatment of cutaneous leishmaniasis[2,3]. The nanoparticles were synthesized via a controlled chemical route, involving the formation of a silver core followed by gold coating, resulting in core–shell bimetallic structures[3]. UV–Vis spectroscopy revealed plasmonic absorption bands between 300 and 600 nm, attributed to metallic silver and gold (Figure 1). Dynamic light scattering (DLS) analysis indicated a hydrodynamic diameter of approximately 63 nm, confirming the formation of nanometric structures. The nanoemulsions were formulated using Tween 80 (5 or 10%) as surfactant and sunflower oil or lemon essential oil as the oil phase, processed by Ultra-Turrax® homogenization or probe ultrasonication, and are under parameterization for subsequent incorporation of Ag@AuNPs, aiming to evaluate physicochemical compatibility, hybrid system stability, and suitability for topical application.

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UV–Vis spectrum of AgNPs (green line) and Ag@AuNPs (blue line)

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Development of Nanostructured Sensors for Cancer Diagnosis

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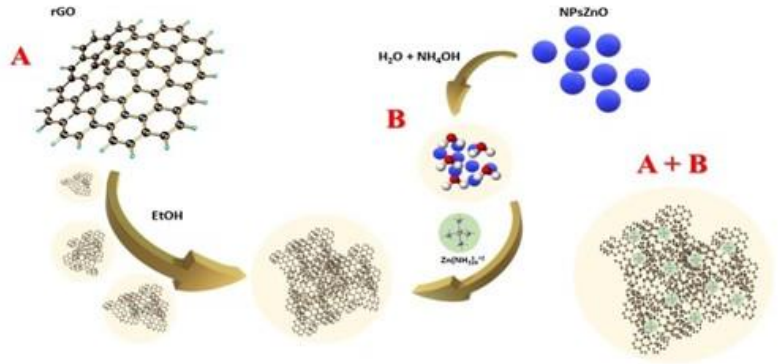
Palavras Chave:*Cancer, Biosensor, Graphene, Screen Printing, Graphene Oxide.,Cancer, Sensor, Graphene, Screen Printing, Graphene Oxide.*

Highlights

Nanostructured graphene-based electrodes were developed for electrochemical sensing. Samarium oxide significantly enhanced the electrochemical response of the sensor.

Resumo/Abstract

Cancer develops from the uncontrolled proliferation of cells. In most cases, this disease lacks efficient screening methods and typically presents an aggressive progression. Therefore, the development of biosensors emerges as a promising alternative for early cancer detection. The objective of this study was to evaluate the construction of new electrochemical devices and their analytical application. Two electrode models containing reduced graphene oxide in their matrix were fabricated. The first was prepared by modification with samarium oxide using a hydrothermal technique, while the second was produced via screen-printing using conductive graphene ink. An electrochemical cell was fabricated by 3D printing using AutoCAD slicing software, followed by assembly of the printed components. Initial prototypes exhibited electrolyte leakage; therefore, subsequent prints were optimized by adjusting layer density to ensure better sealing. Graphene paste, zinc oxide, and mineral oil were then incorporated, resulting in signal generation analyzed using Nova 2.0 software. Analytical application was performed through dopamine testing using the graphene/zinc oxide electrode, which showed a satisfactory analytical response. After confirming the expected response, samarium was added to the electrode, leading to a significant increase in the analytical curve and current response. Finally, graphene-based electrochemical sensors were prepared using screen-printing technology with defined molds, onto which conductive graphene paste was deposited, enabling the development of a new sensor using graphene ink. The development of new electrochemical platforms demonstrated significant results in the detection of analytes correlated with cancer, indicating high potential for the development of new biosensors for the specific detection of antigens associated with different types of cancer.



Illustrative scheme of the synthesis procedures for the rGO/Sm_2O_3 nanocomposite

Agradecimentos/Acknowledgments

The authors thank FAPEMA and Universidade CEUMA for financial support and laboratory infrastructure, and acknowledge all collaborators involved in the development and evaluation of the electrochemical biosensors.

Dialysis-induced structural and photonic fractionation of carbon dots

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Palavras Chave:*Carbon dots,Purification,Surface chemistry,Photoluminescence*

Highlights

Optical variability increases in high energy synthesis.
Post-synthetic purification is critical to controlling electronic structure
Dialysis induced spectral changes and size fractionation

Resumo/Abstract

Carbon dots (CDs) have attracted increasing attention due to their tunable photoluminescence, low toxicity, and broad applicability in sensing, catalysis and agriculture due to their ability to modulate physiological processes in crops. However, achieving consistent optical properties across different studies remains challenging, partly due to variations in synthesis routes and post-synthetic purification procedures. Dialysis is widely used to remove low-molecular-weight species, although factors such as membrane molecular weight cut-off (MWCO) and dialysis time are not always explored in terms of their potential impact on the material's properties. In this work, CDs derived from citric acid and urea were synthesized via microwave-assisted hydrothermal route under different temperatures (160 and 200 °C), reaction times (25 and 45 min), and precursor ratios (1:4 and 1:2.25, acid:urea). Optical properties were evaluated after dialysis (1 kDa MWCO, 48 h) by excitation–emission spectroscopy and relative quantum yield with quinine sulfate as standard, revealing that higher temperatures and longer reaction times led to increased variability, attributed to enhanced carbonization and formation of heterogeneous emissive populations. The condition with the lowest variability (1:4, 200 °C, 25 min) and higher quantum yield was selected for a systematic study of dialysis time (24–120 h). Time-resolved purification induced pronounced spectral changes indicating a progressive redistribution of emissive states. Transmission electron microscopy revealed size fractionation. These observations demonstrate that a 1 kDa membrane does not promote simple purification but rather a time-dependent structural and photonic fractionation process. These findings highlight that post-synthetic purification is critical to controlling electronic structure, optical behavior, and reproducibility, and therefore must be considered an integral part of CD synthesis rather than a merely technical step.

Agradecimentos/Acknowledgments

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DODECYL ESTERS FROM SMA AS ANTIFREEZE POLYMERIC ADDITIVES FOR BIODIESEL

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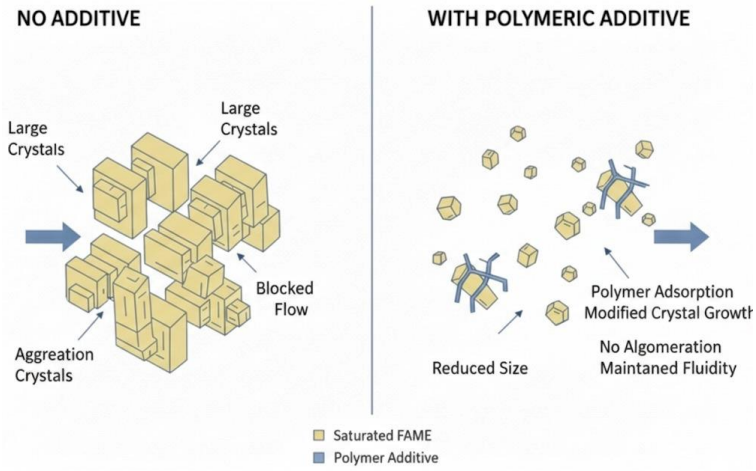
Palavras Chave:*SMA,Poly(styrene-co-dodecyl maleate),Antifreeze polymeric additives,Biodiesel,Pour point*

Highlights

Dodecyl polymeric esters, derived from SMA, reduce the pour point of soybean methyl biodiesel (B100) from -3 °C to -31 °C, improving cold performance and fuel stability.

Resumo/Abstract

Among the actions needed to slow down the undeniable climate change are the increase and diversification of clean and sustainable energy sources. Despite advances in the development of new biofuels, biodiesel still proves to be an excellent alternative to petrodiesel. The increase in the share of biodiesel in the Brazilian energy matrix has stimulated the diversification of raw materials, including those of low quality and low added value, as well as the development of additives to improve the properties of these biofuels. Unlike most of Brazil, the states in the southern region of the country are subject to low temperatures for a large part of the year, which impairs the operation of equipment, power generators and engines powered by diesel oil and/or biodiesel, as such fuels tend to gradually solidify with the reduction of ambient temperature. Polymeric esters have been used as additives in the petroleum industry, but little explored as additives for biofuels. To improve the cold flow properties of biodiesel, in this work polymeric additives capable of reducing the pour point (PP) of soybean methyl biodiesel (B100) were developed. Styrene and maleic anhydride copolymers (SMA) were synthesized under varying conditions, which were later esterified with 1-dodecanol to produce antifreeze polymeric additives. The composition of the copolymers, degree of esterification and structural characterization were performed by FTIR, ^{1}H and ^{13}C NMR, GPC and neutralization volumetry. The excellent antifreeze activity of the different poly(styrene-co-dodecyl maleate) copolymers was proven by the reduction of PP of soybean methyl biodiesel (-3 °C) with only 1000 ppm added. Copolymers containing 20 to 27 mol% of esterified units showed the greatest PP reductions, reaching values in the range of -25 °C to -31 °C.



Pictorial representation of the mechanism of action of antifreeze additives.

Agradecimentos/Acknowledgments

CAPES, CNPq, PPGQ/UFPR, INT-RJ/MCTI, RBTB/MCTI, UFPR, DQUI/UFPR, LabRMN/UFPR.

Eco-Friendly Synthesis of Au-Pd Bimetallic Nanoparticles Using Alpinia zerumbet for Efficient Reduction of Nitro Compounds

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Palavras Chave:*Green synthesis,Au–Pd nanoalloys,Alpinia zerumbet,nitroaromatic reduction,sustainable catalysis*

Highlights

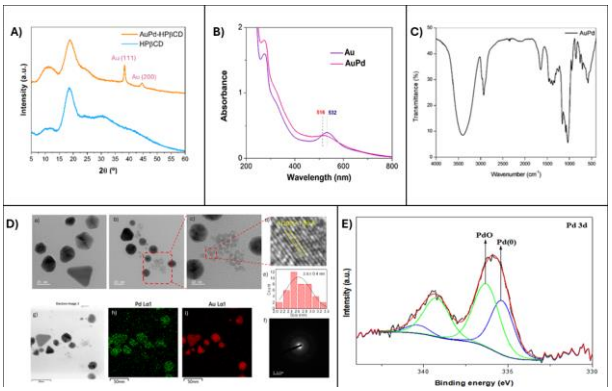
• Sustainable Au–Pd nanoalloys were synthesized using plant extract and cyclodextrin as stabilizer.

• Au–Pd nanoparticles showed strong synergistic catalytic effect in nitroaromatic reduction in water.

Resumo/Abstract

Catalytic hydrogenation of nitroaromatics is a convenient transformation for the production of high value-added amines and, simultaneously, an alternative route for the remediation of toxic and potentially carcinogenic pollutants. Bimetallic Au–Pd nanocatalysts stand out for their high activity and selectivity, attributed to electronic and structural synergistic effects. However, conventional synthetic routes for these materials employ aggressive and environmentally harmful reagents, compromising the sustainability requirements. In this work, we propose a green route for the synthesis of Au–Pd nanoalloys using*Alpinia zerumbet*extract as both reducing and stabilizing agent, in combination with 2-hydroxypropyl-β-cyclodextrin. Phenolic phytochemicals present in the extract promoted the bimetallic nanoparticle formation and stabilization without the need for toxic additives.

Combined characterization by XRD, HRTEM/EDS, XPS, DLS, and UV–Vis spectroscopy provided consistent evidence for the formation of bimetallic nanostructures with alloy-like features, exhibiting a bimodal size distribution and ultrasmall nanoparticles with an average size of 2.6 ± 0.4 nm. Zeta potential measurements indicated enhanced electrostatic stabilization in the bimetallic system. Catalytic performance revealed a strong synergistic effect between Au and Pd: while Au nanoparticles exhibited nearly negligible activity and Pd showed only moderate conversion, the Au–Pd system achieved near-quantitative yields in nitrobenzene reduction within only 15 minutes. In this case, we obtained TOF values up to 393 h^{-1}, surpassing reported systems that required harsher conditions. The catalyst also demonstrated efficiency in the reduction of 3-nitroaniline and 4-nitrophenol with high selectivity. These results demonstrated that integrating plant extracts with supramolecular systems enables the development of efficient, robust, and environmentally sustainable nanocatalysts.



Characterization of AuPd Nps: A) XRD; B) UV–Vis; C)FT-IR ; D) TEM/HRTEM/SAED/EDS and E) Pd 3d XPS.

Agradecimentos/Acknowledgments

We acknowledge UERJ, Van de Graaff Lab - PUC-RIO, FAPERJ (CNE 2021: E-26/200.416/2023), CNPq (PQ-2/2021: 316550/2021–3) and CAPES – Brazil (Finance Code 001) for financial support.

Efeito sinérgico entre a casca oriunda da Lucina pectinata calcinada e a biomassa matriz Cola acuminata – Avaliação e desempenho

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Palavras Chave:*Cola acuminata; Lucina pectinata, analise termogravimétrica; Py-GC-MS.*

Highlights

Calcinated*Lucina pectinata*alters*Cola acuminata*pyrolysis, increasing CaO crystallinity, thermal stability and promoting deoxygenation, yielding more aromatic vapors and stable biochar.

Resumo/Abstract

A pirólise de biomassas lignocelulósicas tem se mostrado uma estratégia promissora para a valorização de resíduos. Neste estudo, avaliou-se a influência da adição de uma segunda biomassa (*Lucina pectinata*)-L calcinada a 850°C para atuar como reforço na biomassa matriz (*Cola acuminata*)-C nas proporções mássicas CL(1:1, 1:2 e 1:3) onde foram maceradas por 10 min gerando as simbologias CL1, CL2, CL3. As amostras foram caracterizadas DRX, EDX, TG, e Py-GC-MS. Os resultados de DRX indicaram que a*Cola acuminata*apresenta um halo amorfo em 2f =21°indicando a presença de celulose do tipo I. Após adição de L, nas proporções indicadas pode-se notar que a medida que aumentamos a relação L:C os halos tornam-se mais cristalinos tendendo para a forma cubica do óxido de cálcio (01-077-2010) diminuído a intensidade da presença da celulose. Esses resultados, estão em concordância com o EDX apresentado pois os teores de cálcio são alterados de 52,15% da biomassa C para 98,02% para a mistura CL3. As curvas TG indicaram três estágios de perda de massa com a formação de uma pseudo-fase estacionária em 700°C independente do aumento da proporção em L. Os resultados de Py-GC-MS mostraram que a presença de L altera a composição dos vapores pirolíticos. As amostras CL1 e CL2, apresentou similaridades nos seus teores, enquanto CL3, conduziu ao aumento relativo de compostos aromáticos menos oxigenados. Esse comportamento indica que a atuação da*Lucina*calcinada, promove reações de desoxigenação, desmetoxilação e craqueamento secundário dos vapores. De forma integrada, os resultados demonstram que um novo composto é gerado pelo efeito sinérgico entre a*L. pectinata*calcinada e a biomassa matriz, favorecendo a obtenção de um biocarvão com maior estabilidade térmica, formação de produtos de maior valor agregado, ampliando o potencial da biomassa para aplicações energéticas e ambientais.

Agradecimentos/Acknowledgments

A Yalorixa Lucia de Oliveira (Omidewá) do terreiro Ylé Axè Opô Omidewá por permitir a coleta das casas do Cola acuminata, a Universidade do Estado da Bahia (UNEB), Fundação de Amparo à Pesquisa da Bahia (FAPESB) e ao CNPq pela concessão das bolsas.

Effect of Calcination Temperature on Cu-Functionalized NiFe LDHs and Derived Oxides in the Catalytic Reduction of 4-Nitrophenol

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Palavras Chave:*LDH, LDO, Catalytic Reduction, Magnetic, 4-Nitrophenol*

Highlights

CuNiFe-LDHs were synthesized and calcined at 400 and 600 °C.

Magnetic materials were obtained without additional magnetic components.

CuNiFe-LDH calcined at 600 °C reduced 4-NP in 25 s.

Resumo/Abstract

Layered double hydroxides (LDHs) and their derived oxides (LDOs) have been investigated as heterogeneous catalysts, especially in catalytic reduction reactions for environmental remediation, due to their high surface area, tunable lamellar structure, low cost, and chemical modifiability[1]. These materials exhibit a memory effect, enabling reconstruction of the lamellar structure after calcination when in contact with ion-containing solutions[2]. Calcination may also generate magnetic phases, facilitating catalyst recovery and reuse. In this study, a NiFe-based LDH was synthesized and calcined at 400 °C and 600 °C to obtain the corresponding oxides. The oxides were reconstructed in an aqueous Cu^{2+} solution, followed by a second calcination and $NaBH_4$ reduction to activate metallic species. The effect of thermal treatment was evaluated in the $NaBH_4$-mediated catalytic reduction of 4-nitrophenol (4-NP), a toxic compound used in dyes, pesticides, and chemical intermediates, into 4-aminophenol, an intermediate for paracetamol synthesis[3]. X-ray diffraction confirmed LDH reflections and crystalline phases related to magnetic behavior, while elemental mapping confirmed copper incorporation. Catalytic results showed that LDH-CuNiFe calcined at 600 °C presented the highest apparent rate constant (*kapp*= 27.1 min^{-1}, ~0.25 min), whereas the corresponding oxide showed lower performance (*kapp*= 4.9 min^{-1}, ~1.1 min). At 400 °C, LDH-CuNiFe reached*kapp*= 12.9 min^{-1} (~1.2 min) and LDO*kapp*= 1.5 min^{-1} (~2.5 min). Overall, LDHs outperformed LDOs, and higher calcination temperatures improved catalytic activity and magnetic behavior. Future studies will evaluate stability, reusability, and the reduction of other nitrocompounds to assess substituent effects on catalytic efficiency.

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Agradecimentos/Acknowledgments

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EFFECT OF CARBODIIMIDE MOLAR MASS ON THE CHAIN EXTENSION OF POLYAMIDE 6

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Palavras Chave:*Polymer recycling,polyamide 6,chain extension,carbodiimide,polycarbodiimide*

Highlights

Changes in PA6 chain extension during the recycling process due to variations in the molar mass of carbodiimide.

Resumo/Abstract

The versatility of polymeric materials has led to their large-scale production, making them essential for several industrial sectors. Among them, polyamide stands out due to its wide range of applications, from the automotive to the textile industries, reaching a global production of approximately 5.58 million tons in 2019. However, plastics have become an environmental concern due to the linear economic model, which leads to increased disposal, landfill accumulation, and greenhouse gas emissions. In this context, recycling becomes a viable alternative. In the case of polyamide 6 (PA6), a condensation polymer, it is susceptible to hydrolysis reactions during reprocessing, leading to molar mass (MM) reduction and changes in molar mass distribution (MMD), resulting in alterations in the physicochemical properties that hinder its reintegration into the same production cycle or into applications with higher added value. One strategy to overcome this limitation is the use of carbodiimides (CDIs), which act as anti-hydrolysis agents and chain extenders during PA6 recycling. Since CDIs with different MM may behave differently during PA6 processing, this work investigates the influence of CDI MM on the PA6 chain extension efficiency. A monomeric CDI (Stabaxol I, Lanxess) and an oligomeric CDI (PCDI, Stabaxol P, Lanxess) were evaluated. PA6 (RADILON S 40F 100NT, Radici) was processed in a co-rotating twin-screw extruder using 0%, 1.5%, and 3% of each additive. Rheological analyses showed increased viscosity with both CDIs, with a more pronounced effect for PCDI, indicating higher chain extension efficiency. Samples containing PCDI also exhibited a less pronounced increase in pseudoplastic behavior, suggesting smaller changes in MMD. DSC results showed a reduction in crystallization temperature for PCDI, while mechanical tests indicated higher elongation at break. These findings demonstrate that CDIs with higher MM are more effective in PA6 chain extension.

Agradecimentos/Acknowledgments

We acknowledge FAPESP (2023/07174-6 and 2025/12536-0) for financial support, and the Department of Chemistry and the Graduate Program in Chemistry at the Federal University of São Carlos (UFSCar) for scientific and institutional support.

Effect of grinding on the structure, composition, morphology and size of biochars

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Palavras Chave:*: Biomass, carbonaceous materials, ball mill, nanobiochar, Raman,Biomass,Carbonáceos Materials,Ball mill,nanobiochar,Raman espectroscopy*

Highlights

Biochar is prepared by thermal treatment in static air atmosphere and ground in a high-energy ball mill; Samples showed a greater number of defects, superficial oxidation and submicron particle sizes.

Resumo/Abstract

Biochars are widely studied carbon-based materials with applications in environmental remediation, soil conditioning, and electrochemical sensors. High-energy ball milling allows particle size reduction of biochars to the ultrafine or nanometric scale, improving material performance. In this work, a biochar produced from sugarcane bagasse by thermal treatment in static air atmosphere (muffle furnace, 500 °C, 1 h) and milled (Pulverisette 6, Fritsch) under different conditions was characterized in terms of composition, structure, morphology and size to evaluate the effects of milling. A 2^3 experimental design with a central point, varying the milling time (1–2 h), rotation speed (150–300 rpm), and the mass ratio of spheres/biochar (20:1–50:1) was carried out. The central point was at 1.5 h, 230 rpm, and 35:1. The ground biochars showed a slight increase in carbon content compared to raw sample (CHNS analysis). XPS spectra revealed the presence of C, O, K, and Si in the samples, and no contamination was detected from the grinding equipment. An increase in the atomic quantity of O1s was observed after grinding, indicating superficial oxidation, with oxygen content increasing from 12.6% in the raw sample to 18.3% in the grounded one for 2 h, 300 rpm, and 50:1 mass ratio. FTIR spectra showed band broadening between 1700 and 1600 cm^{-1}, attributed to C=O stretching, corroborating the XPS results. Raman spectra exhibited an increase in the ID/IG ratios and an increase in area for the band at 1180 cm^{-1}, indicating both higher density of defects and amorphous carbon content. SEM analysis showed that bulk biochar exhibited a fibrous morphology with particles larger than 1 µm, while milled samples displayed irregular shapes and reduced particle sizes, ranging from 0.08 to 0.75 µm. These results demonstrate that high-energy milling induces significant changes in the composition, structure, and morphology of biochars, which is crucial for future applications.

Agradecimentos/Acknowledgments

To CAPES for the scholarship and research financial support (Code 001), National Council for Scientific and Technological Development (CNPq) and State university of Londrina (UEL).

EFFECT OF H2O2 DOSAGE ON THE DECOLORIZATION OF CRYSTAL VIOLET DYE BY THE HETEROGENEOUS FENTON PROCESS USING A LOW-COST CATALYST.

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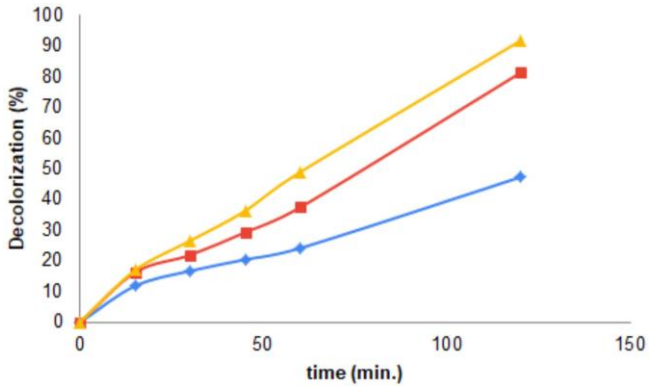
Palavras Chave:*Azo dyes,Coffee husks,Sustainability,Water resources.*

Highlights

Low-cost catalyst was active in the removal of crystal violet dye by the Heterogeneous Fenton Reaction. Generating new products with higher added value from agro-industrial waste.

Resumo/Abstract

The growth of industrial activities has led to an increase in waste generation, which is often disposed of in the environment without proper treatment. Many methods have been proposed, but they present several limitations – mainly related to the cost and efficiency of the treatments. Advanced oxidation processes have been applied with great effectiveness in wastewater remediation, among which the Heterogeneous Fenton Process stands out. In this work, a catalyst based on iron oxide supported on hydrochar produced from coffee husks was obtained and applied to the decolorization of crystal violet dye through the Heterogeneous Fenton Process.The catalyst was synthesized from the precipitation of iron particles in the hydrochar structure using sodium borohydride followed by calcination at 500 °C. The material was characterized by Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). For the catalytic tests, an aqueous solution of crystal violet dye was used as a model pollutant in the presence of the catalyst and with different aliquots of H_2O_2. The FTIR spectrum exhibited vibrational modes typical of aromatic structures and oxygenated functional groups. The X-ray diffraction pattern revealed an amorphous halo and diffraction peaks characteristic of hematite. The decolorization rate varied with the amount of hydrogen peroxide used. After 120 minutes of reaction, the efficiency was observed to be 47%, 81%, and 92%, respectively, for aliquots of 1 mL, 2 mL, and 3 mL of peroxide. The kinetic data of the catalysts were fitted to first- and second-order kinetic models. Based on the correlation coefficients found, it was verified that the results best fit the first-order kinetic model. The low-cost catalyst produced was efficient for removing crystal violet dye from aqueous media using a Heterogeneous Fenton Process, contributing to the reuse of waste with no commercial value, as well as to the treatment of wastewater contaminated with azo dyes.



Effect of H_2O_2 dosage on the removal of crystal violet dye by the Heterogeneous Fenton Reaction

Agradecimentos/Acknowledgments

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Effect of lignin and hemicellulose content on the microstructure and oil absorption performance of sugarcane bagasse nanocellulose-based cryogels.

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Palavras Chave:*Nanocellulose,Cryogels,Sugarcane bagasse,Oil absorption,Oil absorption kinetics*

Highlights

Nanocellulose cryogels were produced from sugarcane bagasse; Biomass composition controlled cryogel microstructure; Higher cellulose content increased soybean oil absorption.

Resumo/Abstract

Oil spills (both mineral and vegetable) are responsible for a great part of long-term water pollution, underscoring the need for efficient and sustainable cleanup methods. In this work, different nanocellulose cryogels were produced by chemically treating sugarcane bagasse in order to modulate lignin and hemicellulose content. To evaluate the microstructure and fibrillation degree, the materials were characterized by X-ray microtomography (MicroCT) and atomic force microscopy (AFM), and the oil absorption capacity was assessed using soybean oil. MicroCT analysis revealed highly porous structures (>95%) with average pore diameters ranging from approximately 278 to 337 µm, depending on chemical treatment. Cryogels with higher cellulose content exhibited thinner pore walls, predominantly distributed in the 8–24 µm range, whereas lignocellulosic cryogels showed thicker walls mainly between 24–40 µm. The progressive removal of lignin and hemicellulose promoted enhanced mechanical fibrillation, leading to more homogeneous porous structures. As a result, sugarcane bagasse-derived cryogels exhibited oil absorption capacities of 33 ± 3 g g^{-1}, with faster absorption rates for the cryogel richer in lignin. These results demonstrate that the microstructure is key to oil absorption, highlighting sugarcane bagasse-derived nanocellulose cryogels as promising renewable absorbents for vegetable oil spill remediation.

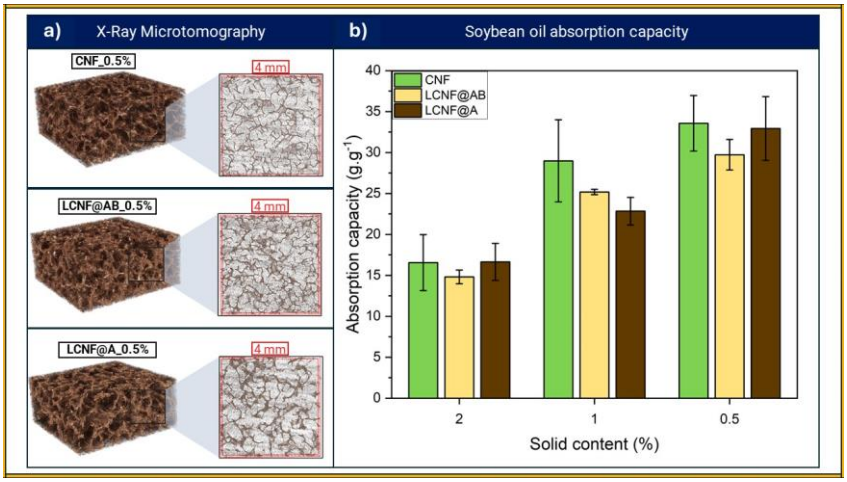


Figure 1. (a) X-ray microtomography images and (b) soybean oil absorption of nanocellulose cryogels.

Agradecimentos/Acknowledgments

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Effects of ion migration on the crystalline structure of MAPI thin films with varying surface defects density

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Palavras Chave:*Hybrid organic-inorganic perovskites, solar cells, ion migration, nano-XRF mapping, nano-XRD*

Highlights

Ion migration in perovskites degrades solar cell performance Chemical distribution was investigated using nano-XRF mapping Phase composition was evaluated by nano-XRD

Resumo/Abstract

Hybrid organic-inorganic perovskites represent one of the most promising emerging photovoltaic technologies, demonstrating remarkable development in just over a decade. Their PCE has soared from 3.8% in the first reported device in 2009 to values exceeding 25%, rivalling well-established silicon solar cells. Despite these impressive efficiency gains, challenges persist in achieving commercial viability, particularly in terms of long-term stability and scalable manufacturing. One major obstacle is the movement of ions within the material during device operation, which can lead to many harmful effects on solar cells. Understanding the factors that influence ion migration is therefore crucial for designing more stable and efficient devices. The density of surface defects has been shown to significantly impact the performance and stability of perovskite photovoltaic devices, suggesting that ion migration may also be affected by this factor. In this work we investigated how the crystalline structure changes due to ion migration, particularly involving iodide ions, and how varying the density of surface defects, achieved through slight adjustments in the I/Pb ratio in $MAPbI_3$ films, can influence these changes. To accomplish this, we assessed the chemical distribution and phase composition in a sample area subjected to a constant electric field to stimulate ion migration using nano-probe synchrotron-based techniques such as X-ray Fluorescence (XRF) and X-ray Diffraction (XRD) at LNLS-SIRIUS. The results suggested that the increased density of interstitial iodine defects expected for MAPI 3.04 (above the stoichiometric value) influences iodine migration when subjected to an electric field of 0.15 V μm^{-1}. This sample appears to exhibit enhanced resistance to halide migration and, consequently, to film degradation. Overall, this new approach provides deeper insight into the key factors governing ion migration, opening new pathways for improved material stability.

Agradecimentos/Acknowledgments

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Effects of nanocelluloses and pectins in aqueous foam stability

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Palavras Chave:*Foams, Nanocellulose, Pectin, Biopolymer, Stability*

Highlights

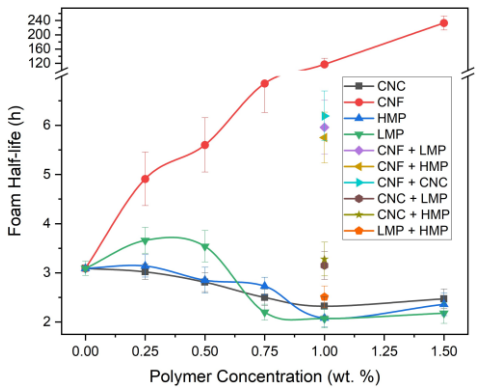
Foams prepared with surfactant and biopolymers within a range of concentrations

Foam half-life was enhanced to more than a week with nanocelluloses

Highly-stable foams reinforced by calcium cross-links

Resumo/Abstract

Aqueous foams are gas dispersions in liquid, used in various sectors, such as food, cosmetics and cleaning. Despite being thermodynamically unstable systems, aqueous foam lifetime can be increased by adding colloids and thickeners, such as polymers and nanoparticles, which reduce coarsening, drainage, and coalescence. In this work, cellulose nanocrystals and nanofibrils (CNCs and CNFs) and high and low-methoxyl pectins (HMP and LMP), renewable and biocompatible biopolymers, were used to assemble aqueous foams with 0.5% (m/m) sodium dodecyl sulfate (SDS). The systems were prepared with different biopolymer concentrations (0.25 - 1.5%), obtaining dispersions with negatively charged colloids and pseudoplastic behaviour. The foams were prepared by mechanical agitation, and their foamability, bubble size and half-life time (t ½) were determined. The results indicated that foamability and bubble size were inversely proportional to biopolymer concentration, due to increased viscosity, which led to less air incorporation. The incorporation of 1.5% biopolymer reduced the original average bubble size (397 µm, SDS only) to 182 µm for CNC, 144 µm for CNF, 124 µm for HMP, and 124 µm for LMP. The durability of the foams was extended with HMP, LMP, and CNFs, with t ½ increasing from 3.15 h without biopolymers to 233 h (1.5% CNF). On the other hand, CNCs did not provide greater stability, suggesting that increased viscosity was not the only relevant parameter. The combination of biopolymers increased the t ½ in all cases compared to the same concentration of a single polymer, demonstrating synergic effects. Cross-linking with calcium ions proved efficient at enhancing the stability of all systems (1.5% biopolymer), forming resistant gels as calcium ions interacted with the biopolymer's negative groups. Thus, this study points to a green way to increase the durability of foams using plant-based colloids, with potential application in cosmetics and food.



Half-life of foams with SDS and biopolymers. Multicomponent systems have 0,5% of each biocolloid.

Agradecimentos/Acknowledgments

FAPESP through the Young Investigators Grant (23/09659-7), and the Research, Innovation and Dissemination Center for Molecular Engineering for Advanced Materials – CEMol (Grant CEPID No. 2024/00989-7). GGS thanks the scholarship FAPESP 2024/17802-7.

Electrodeposited Zn-Co electrocatalysts for hydrogen evolution reaction

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Palavras Chave:*Hydrogen evolution reaction, electrocatalyst, metallic alloys ,electrodeposition, thin films*

Highlights

Bimetallic electrocatalysts for hydrogen evolution reaction.
Direct electrodeposition from aqueous solutions.
Amorphous Zn-Co alloys.

Resumo/Abstract

Hydrogen is a rising use energy source alternative to fossil fuels, which demands different routes for its generation. Green hydrogen can be obtained through water electrolysis, a method for which good catalysts are required to achieve efficiency and cost reduction. In this work, Zn, Co and Zn-Co alloys were electrodeposited from aqueous solutions on Cu substrates. The obtained films were used as electrocatalysts for the hydrogen evolution reaction (HER) in acid solution (pH = 4). The potentiostatic deposition process has been done at room temperature in a conventional three-electrode cell with $CoSO_4$, $ZnSO_4$, and H_3BO_3 (pH = 3). An*in situ*quartz microbalance has been used for the measurement of the deposited mass. The results for different concentrations of the reagents, additives and applied potentials were investigated. Cyclic voltammograms and chronoamperometric curves were recorded. The HER was evaluated considering potentiometric curves between –1.1 and –1.7 V (vs. Ag/AgCl), as well as chronoamperometric curves in $(NH_4)_2SO_4$. A representative example is shown in Figure 1. The composition of the samples was determined before and after the HER tests by means of energy dispersive spectroscopy (EDS). Scanning electron microscopy (SEM) was used for the assessment of the samples morphology, and x-ray diffraction for the structure. The structure of the samples tends to be crystalline for the pure metals, but amorphous for the alloys. The alloys with low content of Co (~16 at.%) present the largest efficiency for the HER (1.09 10^{-6}mol $cm^{-2}s^{-1}$). More negative is the applied potential for the deposition, larger is the amount of hydrogen generated. The EDS results show that a partial oxidation of the electrocatalyst films occurs during the procedure of H_2 generation. The chronoamperometric curves present an approximately stationary behavior after a transient interval from 3 to 20 s at –1.4 V.

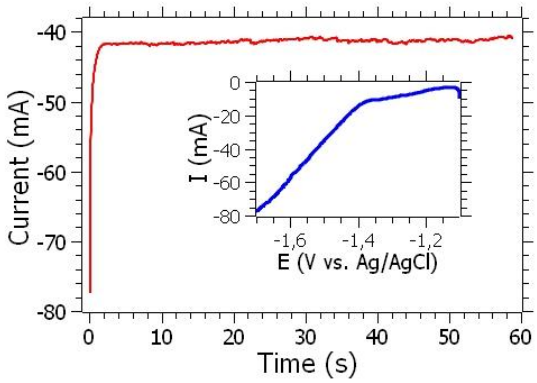


Figure 1. Chronoamperometric and potentiometric curves for a Zn-Co film.

Agradecimentos/Acknowledgments

Work supported by FAPEMIG (Projects APQ-00370-22 and APQ-02562-24). Lamine Ianga is a CAPES grantee through the GCUB Program for International Mobility. Giovani P. Carvalho is a FAPEMIG grantee (BIS-00410-25).

Electrophilic Susceptibility of Graphene Quantum Dots: Hypochlorous versus Hypobromous Acids—Experimental and Theoretical Study

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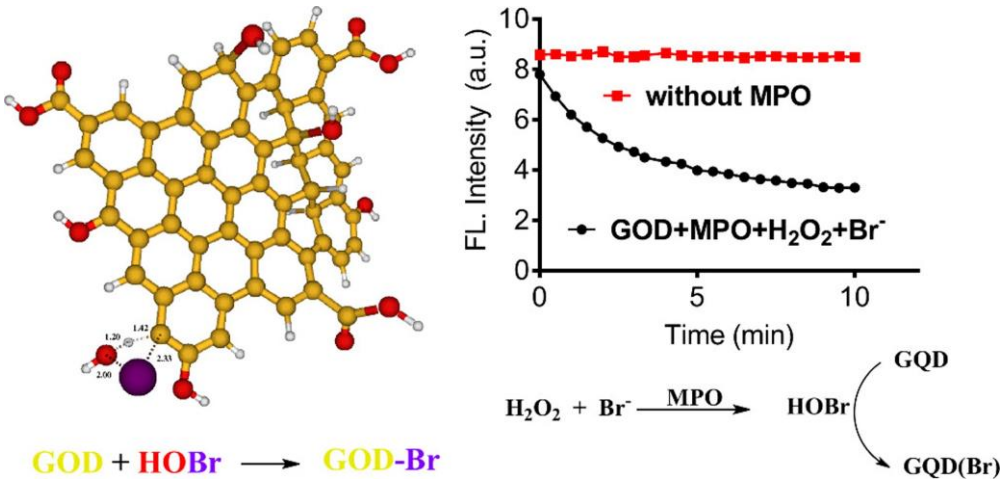
Palavras Chave:*Fluorescência,Pontos Quânticos,Mieloperoxidase,Reatividade*

Highlights

Graphene quantum dots (GQDs) are water-soluble, are biocompatible, and exhibit low toxicity. By monitoring the fluorescence bleaching of the GQDs, we demonstrated that HOBr is more reactive than HOCl.

Resumo/Abstract

Graphene quantum dots (GQDs) are water-soluble, are biocompatible, and exhibit low toxicity. These properties, along with their adjustable and efficient fluorescent emission, make GQDs valuable for biological applications, particularly as spectroscopic nanosensors. In this context, GQDs have been utilized to detect hypochlorous acid (HOCl). While HOCl is a well-known synthetic disinfectant, it is also naturally produced by the enzyme myeloperoxidase (MPO) in mammals. This heme-peroxidase also catalyzes the production of hypobromous acid (HOBr), a more potent halogenating agent. In our study, we compared the reactivity of HOCl and HOBr with GQDs. By monitoring the fluorescence bleaching of the GQDs, we demonstrated that HOBr is more reactive than HOCl. The increased reactivity was attributed to HOBr's higher electrophilicity. The electrophilic nature of the reaction was further confirmed by introducing nicotine as a chlorination catalyst. Anisole did not inhibit the electrophilic attack, confirming the high reactivity of GODs with HOBr. The enzyme MPO was used to generate HOBr through oxidation of Br– by H_2O_2. Thus, the enzymatic activity of MPO could be monitored by GQDs' fluorescence bleaching, and the efficiency of MPO inhibitors could be evaluated. We applied differential function theory (DFT) methodologies to support our experimental findings, proposing a transition state for the electrophilic attack. Consistent with our experimental results, the energetic barrier for the reaction with HOBr was lower than that for HOCl. Overall, our results indicate the susceptibility of GQDs to electrophilic attacks by hypohalous acids and highlight new opportunities for biological applications.



Monitoring HOCl and HOBr reactions and myeloperoxidase activity using graphene quantum dots.

Agradecimentos/Acknowledgments

Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), Centro de computação científica (NCC/GridUNESP)

Electrospun polymeric nanofiber membranes as functional sealing layers for paper-based analytical devices

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Palavras Chave:*Electrospinning, Polymer nanofibers, Colorimetric sensors, Paper-based sensors,Electrospinning, Polymer nanofibers, Colorimetric sensors,,Paper-based sensors,Electrospinning,Polymer nanofibers,Colorimetric sensors*

Highlights

Electrospun polymer nanofibers improve PAD sealing efficiency.

PLA nanofibers show superior porosity and water stability.

Nanofiber-sealed PADs enhance Griess-based nitrite detection.

Resumo/Abstract

Paper-based analytical devices (PADs) are widely used for detecting chemical species, especially as colorimetric sensors, due to their low cost, simplicity, and portability. However, limitations such as poor sample retention in the reaction zone, low moisture resistance, inadequate capillary flow control, and ineffective sealing still compromise analytical performance, leading to leakage and non-uniform color development. These issues highlight the need to optimize PAD architecture, particularly sealing strategies and fluid management. This work evaluated the use of electrospinning to deposit nanofiber membranes onto paper substrates as sealing layers in PADs. Poly(lactic acid) (PLA), polyacrylonitrile (PAN), and poly(ε-caprolactone) (PCL) were electrospun directly onto commercial papers and tested in device fabrication. The colorimetric response was based on the Griess reaction for nitrite detection. Electrospinning parameters were optimized to control fiber morphology, porosity, and wettability-key factors for sealing efficiency and fluid retention. Physicochemical characterization revealed polymer-dependent behavior upon liquid exposure. The resulting PADs showed higher solution retention in the reaction zones than devices sealed with conventional adhesive tape. Among the polymers, PLA stood out due to its hydrophobicity, high porosity, and structural integrity after water absorption. PAN showed low efficiency in retaining liquid and preventing leakage from the sealing layer, while PCL exhibited satisfactory structural and absorption properties but limitations in electrospun deposition onto paper. Overall, electrospun PLA nanofiber membranes are highlighted as promising materials for sealing and structural control in PADs. The optimized polymer–paper composites are proposed for colorimetric nitrite detection, serving as proof of concept for the use of electrospun nanofibers in advanced paper-based analytical platforms.

Agradecimentos/Acknowledgments

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Electrospun PVC/PANI hybrid membranes prepared by in situ aniline polymerization strategies

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Palavras Chave:*electrospinning,lactate biosensor,hybrid membranes,PVC,polyaniline*

Highlights

Electrospun PVC/PANI membranes fabricated via two*in situ*strategies.
Electrochemical sensitivity to lactate (0–94 mM) in artificial sweat.
Membranes show potential for wearable lactate biosensors.

Resumo/Abstract

This work reports the development and characterization of nanostructured poly(vinyl chloride) (PVC) membranes functionalized with polyaniline (PANI), targeting their application as electrochemical biosensors for the non-invasive detection of lactate in sweat. Hybrid membranes were produced by electrospinning using two distinct*in situ*strategies: (i) polymerization of aniline during PVC electrospinning and (ii) polymerization of aniline directly on the surface of PVC electrospun membranes. SEM and TEM revealed uniform fibrous networks, with morphology varying according to the functionalization approach. FTIR and DSC results confirmed the formation of conductive PANI (emeraldine salt) and its chemical interactions with PVC. DMA analysis showed that the incorporation of PANI enhanced the mechanical stability of the membranes while preserving the flexibility required for wearable applications. Contact angle analysis showed that membranes remained hydrophobic, suggesting PANI did not significantly alter PVC's non-polar nature. Biological functionalization was achieved through immobilization of lactate oxidase (LOx), with successful enzyme attachment confirmed by UV–Vis spectroscopy. PANI-containing membranes demonstrated improved enzyme immobilization efficiency, attributed to the presence of amine functional groups in fiber surface. Electrochemical Impedance Spectroscopy measurements in artificial sweat showed a decrease in RCT with increasing lactate concentration (0–94 mM), indicating sensitivity to the target analyte. However, moderate statistical variability was observed (maximum R^2 = 0.83), likely associated with fiber heterogeneity, hydrophobicity, and non-uniform LOx distribution. Overall, the developed nanostructured PVC/PANI membranes demonstrate promising structural, functional, and electrochemical properties, highlighting their potential for integration into wearable devices for real-time, non-invasive lactate monitoring.

Agradecimentos/Acknowledgments

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Eletrochemical Impedance Spectroscopy Study of PAADDA/QHECE/ZnO Nanocomposite Films

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Palavras Chave:*PAADDA,QHECE,Nanocomposite,ZnO nanoparticles*

Highlights

Novel nanocomposites for electrochemical applications. PAADDA/QHECE/ZnO films were made via casting method. ZnO NPs boosted DC/AC conductivities and optimized electrical properties.

Resumo/Abstract

Polymer nanocomposites are a class of materials having nanoparticles or nanofillers dispersed in the polymer matrix, resulting in enhanced properties as compared to the pristine polymer. The poly(acrylamide-co-diallyldimethylammonium chloride)- PAADDA is a water-soluble, cationic copolymer applied in the petroleum, textile, and chemical industries, as well as in wastewater treatment, cosmetic, and pharmaceutical applications. The quaternized hydroxyethyl cellulose ethoxylate-QHECE is a highly water-soluble cellulose-derived copolymer used in the fabrication of gels and films, membrane separation and ion exchange systems. Zinc oxide nanoparticles (ZnO NPs) are intrinsic semiconductors that exhibit notable antimicrobial properties, thermal resistance, and biocompatibility. Therefore, ZnO NPs are widely employed in the pharmaceutical, cosmetic, and food industries. The aim of this work was to obtain and characterize PAADDA/QHECE/ZnO nanocomposite films for electrochemical applications. The PAADDA/QHECE (70/30 w/w) films containing different concentrations of ZnO (1–3% w/w) were obtained by solution casting. The obtained films were characterized by means of attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), and electrochemical impedance spectroscopy (EIS). ATR-FTIR spectra of PAADDA/QHECE/ZnO films showed there were no major changes in the functional groups of PAADDA and QHECE after incorporation of ZnO. Nyquist plots obtained from EIS studies revealed that the incorporation of ZnO nanoparticles in PAADDA/QHECE films improved the DC (óDC) and AC (óAC) conductivities. The highest values of óDC and óAC were found to the PAADDA/QHECE film with 1% w/w of ZnO. Therefore, in this work, novel nanocomposite films of PAADDA/QHECE/ZnO were obtained and characterized by ATR-FTIR and EIS. Experimental results showed that the incorporation of ZnO into the PAADDA/QHECE film optimized its electrical properties.

Agradecimentos/Acknowledgments

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Recycling of poly(butylene adipate-co-terephthalate) (PBAT): DoE-guided molar mass increase via carbodiimide

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Palavras Chave:*PBAT, recycling, carbodiimide, Design of Experiments, sustainability*

Highlights

- PBAT progressively loses molar mass with recycling.
- Hydrolysis and mechanical stress are key drivers of degradation.
- P-CDI additive enhances stability and preserves chain integrity.

Resumo/Abstract

The progressive phase-out of single-use packaging made from fossil-based polymers, alongside growing initiatives promoting the adoption of biodegradable, compostable, and recycled materials in plastic packaging, has recently gained substantial momentum. In this context, the use of biodegradable polyesters, such as poly(butylene adipate-co-terephthalate) (PBAT), stands out as a significant advancement. Although the concept of recycling PBAT may seem contradictory at first, several factors support this strategy: increasing industrial demand, high production costs of biopolymers, limited availability of renewable resources, slow environmental degradation, and the accumulation of solid residues.

This study systematically investigated the mechanical recyclability of PBAT through controlled reprocessing cycles, focusing on its degradation mechanisms and the stabilizing role of a polymeric carbodiimide (P-CDI). Rheological, thermal, and structural analyses revealed a progressive reduction in molar mass and viscosity with repeated processing, driven by hydrolytic and thermo-mechanical degradation. However, the incorporation of P-CDI promoted chain extension and effectively mitigated hydrolysis, as confirmed by viscosity recovery and the identification of N=C=N functional groups via FTIR.

A Design of Experiments (DoE) approach was used to assess the effects of screw speed, additive concentration, and cycle number. Results showed that additive concentration governs stabilization efficiency, while the number of cycles remains the main degradation factor. These findings highlight reactive extrusion with carbodiimide as a promising route to enhance PBAT recyclability and promote circular use of biodegradable polyesters.

Agradecimentos/Acknowledgments

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Encapsulation of the ethanolic extract of Mimosa Tenuiflora for therapeutic treatments and intravaginal lesions.

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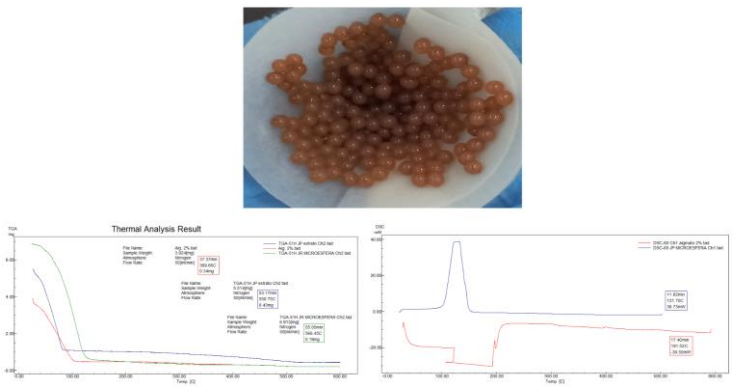
Palavras Chave:*Jurema Preta, antimicrobial, microencapsulation.,Jurema Preta, antimicrobial, microencapsulation,Jurema Preta, antimicrobial, microencapsulation*

Highlights

Development of a therapeutic stick with Mimosa tenuiflora microspheres for the treatment of lesions in the vaginal canal and cervix.

Resumo/Abstract

Jurema Preta (*Mimosatenuiflora*) is a plant found in the northeastern hinterland of Brazil, commonly studied in folk medicine for the treatment of burns, acne, and skin problems, and for its antimicrobial, analgesic, cell-regenerating, and antipyretic properties. Its pharmacological activities are due to the presence of phenolic compounds, such as tannins, found in large quantities in this species. As a phytoactive, it undergoes rapid oxidation. One innovative approach is encapsulation by ionic gelation, an economical and easily reproducible method. This method was used to develop microcapsules containing an ethanolic extract of Jurema Preta. After obtaining the extracts, the microcapsules were characterized by TGA/DSC thermal analysis to evaluate stability and incorporation of the phytoactive. Notably, the ionic gelation encapsulation technique proved to be effective and efficient, ensuring good thermal stability and incorporation of the Jurema Preta extract. In the TGA thermogravimetric curves, the first thermal event (30°C-120°C) corresponds to the loss of residual water mass and volatile compounds. The second event is due to the thermal degradation of the polymeric structure (~200°C). It is observed that the incorporation of the black jurema extract improved the stability of the encapsulated product when compared to alginate. The correlation with the DSC thermogravimetric curves shows the incorporation of the active compounds, a thermal event observed in the encapsulated product containing the black jurema extract, suggesting a chemical interaction of these compounds with the polymeric matrix, confirmed by the alteration of the thermal profile of the original polymer. Overall, the ionic gelation encapsulation technique proved to be effective and efficient, showing itself to be an innovative approach with significant potential to increase the stability and therapeutic efficacy of formulations containing phytoactives.



Microspheres of black Jurema and graphs of the results.

Agradecimentos/Acknowledgments

We thank FAPEAL, CNPq, and FINEP for their financial and institutional support in developing research and strengthening science and innovation in Brazil.

ENZYMATIC SYNTHESIS OF BIOPOLYOLS FOR PRODUCTION OF BIOFOAMS USING AGROINDUSTRY WASTE

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Palavras Chave:*Biopolyol,Glycerolysis,Coffee Grounds,Polyurethane Biofoams,Agroindustrial Waste*

Highlights

Enzymatic glycerolysis of coffee grounds oil produced biopolyols for sustainable polyurethane biofoams.

Different reagent ratios generated biofoams with distinct morphological structures.

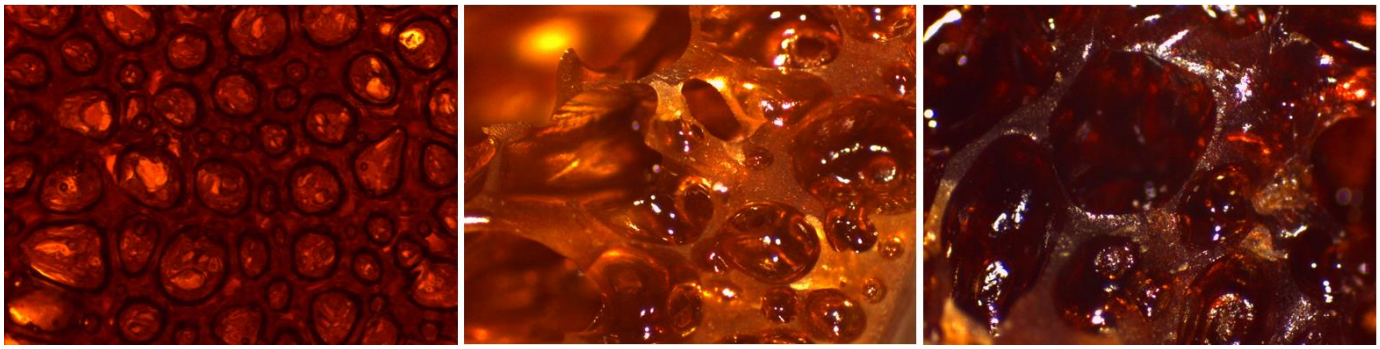
Resumo/Abstract

This study investigates the enzymatic synthesis of biopolyols from coffee grounds oil using glycerol and lipase for production of sustainable polyurethane biofoams. Coffee grounds were dried at 60 °C for 24 h, and the oil was extracted by a reactor-assisted method with ethanol under constant stirring and heating, increasing yield and reducing extraction time compared to immersion extraction.

The oil underwent enzymatic glycerolysis to convert triacylglycerols into mono- and diacylglycerols, generating hydroxyl groups required for polyurethane formation. A Central Composite Design (CCD) was applied to evaluate the best synthesis conditions by analyzing the influence of temperature, glycerol:oil molar ratio, and enzyme concentration. The hydroxyl index was used as the main response variable and showed that the glycerol:oil ratio and enzyme concentration were the most significant factors, while temperature had less influence. The mathematical model presented a high determination coefficient (R^2 = 97.63%), indicating strong agreement between predicted and experimental results.

Biopolyols were characterized by FTIR and hydroxyl index according to ISO 14900:2017 and used to produce polyurethane biofoams with diphenylmethane 4,4-diisocyanate (MDI) at different reagent ratios (1:1, 1:2, and 2:1), resulting in foams with distinct morphological characteristics. The biofoams were further characterized by scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and thermogravimetric analysis (TGA). Digital microscopy enabled evaluation of cell distribution, growth, and homogeneity.

Results show that coffee grounds, an abundant agroindustrial residue, can be valorized through a green enzymatic route to obtain biopolyols suitable for partial replacement of petrochemical polyols. Although ongoing and to be extended to other biomasses, the method shows strong potential for sustainable material development aligned with green chemistry.



Biofoam surfaces photographed with a digital microscope

Agradecimentos/Acknowledgments

We thank FAI UFSCar, IFSP, CNPq, and CAPES for the institutional, scientific, and financial support that made this work possible.

Estratégias para encapsulação de doxorrubicina em nanopartículas híbridas lipídico-polimérica

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Palavras Chave:*Nanoparticles, Doxorubicin, Haluronic Ácid, PLGA, Nanoprecipitation;*

Highlights

Nanopreciptiation method influenced particle diameter and homogeneity; Hyaluronic acid-based formulation showed potential for further studies

Resumo/Abstract

A doxorrubicina (DOX) é um antineoplásico amplamente utilizado na prática clínica, porém apresenta elevada cardiotoxicidade. Nesse contexto, este estudo teve como objetivo desenvolver e caracterizar nanopartículas híbridas lipídico-poliméricas (NHLP) para a encapsulação de DOX. As NHLP foram obtidas por nanoprecipitação seguida de evaporação do solvente, sendo avaliadas diferentes composições e métodos de preparo. As formulações foram caracterizadas quanto ao diâmetro médio (DM), índice de polidispersão (PDI) e eficiência de encapsulação (EE). Inicialmente, NHLP brancas foram preparadas a partir de uma fase orgânica composta por PLGA 75:25 (50 mg), lecitina de soja (25 mg) e acetona (3 mL), adicionada a uma fase aquosa contendo Pluronic® F68 (30 mg) e água (9 mL). Dois métodos foram comparados: no método 1, a fase orgânica foi vertida na fase aquosa sob agitação a 8000 rpm por 15 min; no método 2, foi adicionada por gotejamento sob agitação magnética pelo mesmo período. O método 1 resultou em NHLP com DM de 227 ± 22 nm, enquanto o método 2 produziu partículas significativamente menores (190 ± 22 nm; p = 0,03). Ambos os métodos apresentaram PDI inferior a 0,2, indicando sistemas monodispersos. A DOX (1 mg/mL) foi então incorporada pelo método 2; entretanto, a encapsulação foi insignificante. Assim, adotou-se a estratégia de formação de par iônico com ácido esteárico ou ácido hialurônico. A adição desses ácidos não alterou significativamente o DM das partículas brancas, mantendo valores próximos a 200 nm. Contudo, a incorporação de DOX promoveu aumento do DM para aproximadamente 320 nm, com PDI em torno de 0,3. A formulação contendo ácido hialurônico apresentou valores de D90 inferiores a 100 nm e EE significativamente superior à obtida na ausência desse ácido, indicando potencial para otimização e continuidade dos estudos.

Estudo de materiais de documentos do século XVIII do Museu da Inconfidência

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Palavras Chave:*Tinta ferrogálica, espectroscopia Raman, microscopia eletrônica de varredura (MEV), fluorescência de raios X (XRF)*

Highlights

Crystals of calcium sulfate, aluminum sulfate, and potassium silicate were identified on the ink and paper.

Particles of gold and hematite were found on the ink.

Resumo/Abstract

Dentre as tintas de escrita antigas, destaca-se a tinta ferrogálica. Não há uma datação precisa para o início do uso, porém sabe-se que ela foi utilizada desde o final da Idade Média até a primeira metade do século XX.

Para investigar aspectos materiais da deterioração do papel, das tintas e dos cristais presentes em documentos do século XVIII no Brasil, escolheram-se 171 manuscritos da Série Crime do Fórum da Comarca de Ouro Preto, sob guarda do Arquivo Histórico do Museu da Inconfidência. A seleção deu-se pela integridade material dos manuscritos, que, pelo que se sabe, não passaram por tratamentos de conservação, mantendo, assim, suas características mais próximas das originais (Fig. 1).

Além do estudo histórico da formação da Série Crime e do diagnóstico do seu estado de conservação, 48 documentos que apresentavam cristais na superfície foram submetidos à análise de fluorescência de raios X*in situ*, tanto em pontos de tinta quanto no papel. Foram também retiradas 71 microamostras destes manuscritos para análise por MEV e por espectroscopia Raman.

Esse trabalho apresenta os primeiros resultados desta pesquisa. Nos 142 pontos analisados por XRF foram identificados os elementos Al, Ca, Cl, Cu, Fe, K, Mg, Mn, P, S, Si, Ti e Zn. A análise exploratória dos dados foi realizada por meio da Análise de Componentes Principais (PCA) no Matlab, com o PLS Toolbox. Para a PCA do conjunto completo, 7 componentes principais explicaram 73,83% da variância do modelo. Pelo gráfico de pesos, observa-se que a variável responsável por esta separação são as contagens de Fe, onde se agrupam os pontos de tintas. Este resultado indica que as tintas à base de ferro foram utilizadas na maioria dos manuscritos. Das 30 microamostras analisadas por MEV e espectroscopia Raman, foram identificados diferentes óxidos de ferro, alumínio-silicatos, índigo, carbono amorfo, complexos de taninos com ferro e partículas de ouro.

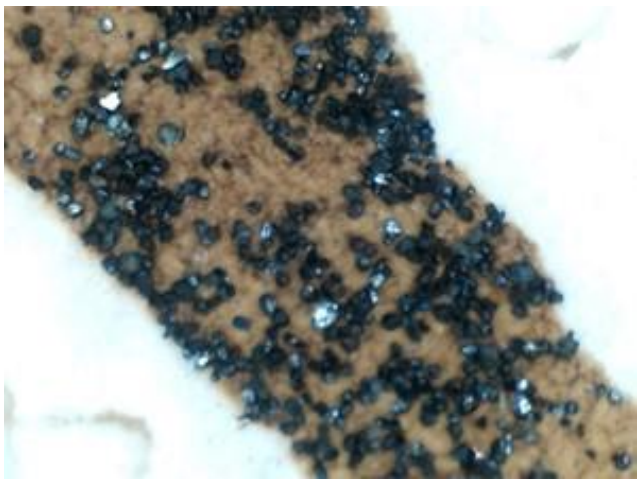


Figura 1: Detalhe da tinta de escrita com cristais de hematita.

Agradecimentos/Acknowledgments

Museu da Inconfidência, Fundação de Arte de Ouro Preto, LCPNano – UFMG, FAPEMIG, UFBA

Estudo exploratório da síntese de zeólitos a partir de resíduos da indústria petrolífera na Bahia.

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Palavras Chave:*Zeólitos,Hidroxicancrinita,Resíduo de perfuração,Tratamento hidrotérmico*

Highlights

Basic treatment of drilling waste makes hydroxycancrinite readily obtainable. The synthesis of zeolite mixtures was possible by using hydroxycancrinite as a source of aluminosilicates.

Resumo/Abstract

Os zeólitos são aluminosilicatos microporosos com ampla aplicação em processos de remediação ambiental , medicina, construção civil, produção de alimentos, adsorção e separação de gases e indústria de catalisadores. A sua obtenção em laboratório envolve, majoritariamente, tratamentos hidrotérmicos em meio alcalino a partir de reagentes puros. O objetivo deste trabalho é investigar a síntese de materiais zeolíticos por tratamento hidrotérmico alcalino utilizando uma mistura de resíduos de perfuração de poços de petróleo como matéria-prima, promovendo a valorização de um material associado a passivos ambientais. Numa primeira etapa, o resíduo foi tratado com NaOH durante 5, 8 e 11 h. Os sólidos obtidos (SC-5h, SC-8h e SC-11h) foram caracterizados por DRX, detectando-se a presença de hidroxicancrinita nos três tempos utilizados. Na etapa seguinte, os sólidos SC-5h, SC-8h e SC-11h foram previamente tratados e submetidos a um processo hidrotérmico a 100 °C por 48, 72 e 120 h para explorar a possível obtenção dos materiais zeolíticos. De acordo com as análises DRX realizadas aos sólidos preparados: i) o tratamento hidrotérmico efetuado sobre SC-5h não gerou sólido cristalino em nenhum dos tempos estudados; ii) no caso das amostras obtidas a partir do sólido SC-8h, não se formou sólido com 48 h de tratamento, no entanto, foi detectada misturas de fases de topologias CHA (fase majoritária) e GIS (zeólito P1) às 72 h e misturas de topologias FAU e GIS (zeólito P1, fase majoritária) após 120 h e por último, iii) utilizando o material SC-11h foi possível obter sólidos cristalinos para os três tempos de tratamento hidrotérmico, formados por uma mistura de fases de topologias FAU e GIS (zeólito P1), a composição percentual das misturas estava na faixa de FAU: 24-36 % e GIS: 64-76 %. O estudo permitiu compreender sobre a possibilidade de preparar zeólitos do tipo FAU e GIS a partir de resíduos de perfuração de poços de petróleo.

Agradecimentos/Acknowledgments

Agradecemos à CAPES, à CNPq, à FAPESB e à FINEP (concessão nº 2427/22) pelo apoio à realização deste trabalho.

Evaluation of acyclovir concentration in electrospun poly(1-vinylpyrrolidone)-co-(vinyl acetate) nonwoven for rapid dissolution

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Palavras Chave:*Rapid Release, Polymer, Drug, Electrospinning,Rapid Release,Polymers,Drug,Electrospinnig*

Highlights

Development of electrospun PVP/VA nonwovens with acyclovir showing reduced crystallinity, improved solubility, and potential for rapid delivery of poorly water-soluble drugs.

Resumo/Abstract

Herpes simplex virus (HSV), especially type 1 (HSV-1), is highly prevalent and causes recurrent orofacial infections. Acyclovir (ACV) is the standard treatment, but its low solubility limits bioavailability. Electrospinning enables the production of nanofibers with high surface area, promoting rapid drug release. The PVP/VA copolymer combines hydrophilic and hydrophobic characteristics that aid in the solubilization and transport of compounds, making it a promising matrix for drug delivery systems. However, few studies have explored electrospun PVP/VA, and none have applied ACV for topical use. This work develops and characterizes ACV-loaded PVP/VA nanofibers, evaluating their physicochemical and morphological properties, as well as their potential for rapid release in the treatment of HSV-1. FTIR analysis revealed interactions between ACV and PVP/VA, evidenced by shifts in the hydroxyl band. ACV increased fiber diameter but improved jet stability, as observed in SEM micrographs, which showed a reduction in beads. XRD indicated that ACV and PVP/VA do not form a fully homogeneous solid solution, as crystalline peaks remained detectable, although with altered crystallinity. DSC confirmed the disappearance of the ACV melting peak in polymer-containing samples. In the Raman spectra, band overlap prevented clear visualization of possible changes. Release kinetics were best described by the Weibull model, with a diffusion-controlled mechanism ($\beta < 1$). Simulated dissolution showed complete solubilization of the electrospun material in 4 s, whereas pure ACV remained undissolved. Overall, the developed system is promising for topical dressings or sublingual fast-release patches for the treatment of HSV-1.

Agradecimentos/Acknowledgments

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Evaluation of Alkaline Fusion and Digestion for LTA Zeolite Synthesis

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Palavras Chave:*Alpha-spodumene,Hydrothermal Syntheses,Zeolite,Alkaline Fusion,Alkaline Digestion*

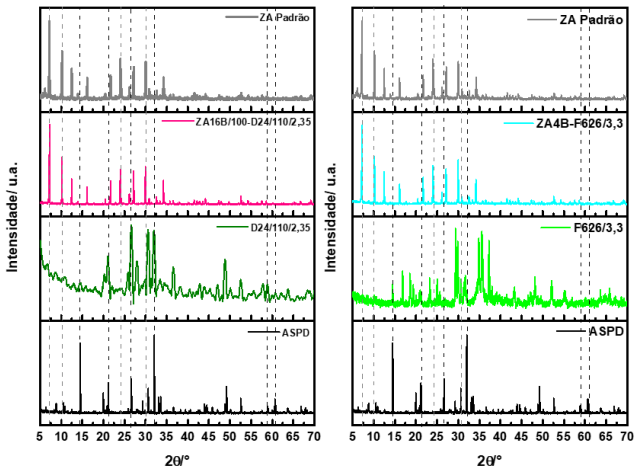
Highlights

LTA zeolite synthesis from α-spodumene alkaline fusion and digestion products was studied. Alkali treatments were optimized using Box–Behnken and factorial designs, and their efficiency was evaluated.

Resumo/Abstract

Zeolites are porous crystalline aluminum silicates with diverse applications. LTA zeolite is more known for its use in ionic exchange, commonly synthesized from ultra-pure reagents. Alpha-spodumene is a lithium aluminum silicate: well explored source of lithium, but only used as a silica source after its conversion into beta-spodumene under high temperatures. This study aims to evaluate the synthesis of LTA through products of both alkaline fusion and digestion of alpha-spodumene, comparing their effectiveness.
The alkaline treatments studied were optimized through different experimental plannings. While the optimization of conditions for the alkaline digestion was passed through box-benhken design, the alkaline fusion was conducted under factorial planning. Through X-Ray Diffraction (XRD), it was possible to define the best conditions for each, which were:
- Fusion under 626°C, with 3.3 grams of NaOH for every 8 grams of spodumene, for 4h;
- Digestion under 110°C, with a NaOH molal concentration of 2.35, for 24h.
Both materials obtained in the optimizations were characterized through XRD, which showed the formation of sodium silicate phases, proving their efficiency in making the crystalline silica available. From both alkaline treated spodumene sources, it was already possible to synthesize LTA, also shown in the diffractograms. Although already having reached the final product (LTA), the precision of this experimental plannings are yet to be determined, currently through the titration of Na_2O and SiO_2 with HCl.

With this, the study shows promise in synthesizing LTA zeolite from an incredibly stable source of silica (alpha-spodumene). The precision of the alkaline treatment must be further developed to make sure that not only the route is sustainable and effective, but also the synthesis is easily reproduceable and up scalable.



XRD Diffractograms of alpha-spodumene, alkaline fusion and digestion, and LTA zeolites synthesized

Agradecimentos/Acknowledgments

Fapemig, CNPq, GruTAm, Labpemol, INCT Midas, Escalab, DQ UFMG

EVALUATION OF PHYSICOCHEMICAL PROPERTIES OF CHITOSAN-BASED FILMS

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Palavras Chave:*chitosan, biodegradability, sustainability, packaging, molecular weight.*

Highlights

The molecular weight of chitosan influences the films' water solubility and water vapor permeability properties. Films formed by high molecular weight chitosan allow more water vapor permeability

Resumo/Abstract

The growing environmental concern has driven the development of packaging from biopolymers. Conventional plastics, widely used in food packaging for their mechanical and barrier properties, have a significant negative environmental impact because they are typically derived from non-renewable sources. To overcome these difficulties, chitosan has been widely explored as a biopolymeric matrix for bioplastic development, owing to its low cost, renewable nature, and commercial availability, as well as its biocompatibility, biodegradability, and interesting physicochemical properties. In this context, the present work aimed to evaluate the physicochemical properties of chitosan-based bioplastics as a function of chitosan's molecular weights (low, medium, and high). The chitosan films were prepared by the casting technique, in which the polymeric matrix (1 g w/v) was solubilized overnight in a 1% (v/v) aqueous acetic acid solution. After this time, glycerol (30% w/w) was added to the film-forming solution and mixed for 5 minutes. The film-forming solution was poured into Petri dishes and subsequently dried in a climate chamber at 35 °C and 45% relative humidity (RH). Chitosan-based films were characterized in terms of thickness, water solubility, water vapor permeability (WVP), and moisture content Regarding to water solubility (%), which was evaluated at low (14.19 ± 1.23), medium (11.39 ± 0.39), and high (12.80 ± 1.16) molecular weight, a significant influence of this parameter was observed ($p < 0.05$). Low molecular weight chitosan films showed greater solubility due to shorter polymeric chains and a less compact matrix, compared to medium- and high-molecular-weight films. Regarding water vapor permeability ($g.mm.m^{-2}.h.kPa^{-1}$), the results applying Tukey's test ($p < 0.05$) show that the films produced with high molecular weight chitosan ($4.63^{-01} \pm 4.40^{-02}$) have higher water vapor permeability values when compared to the low ($3.14^{-01} \pm 1.06^{-02}$) and medium ($2.12^{-01} \pm 1.50^{-02}$) molecular weight chitosan films. This behavior may be associated with greater coiling of the polymer chains with higher molecular weight and the formation of aggregates, resulting in a less homogeneous structure and, consequently, favoring water vapor diffusion. Regarding moisture content (%), the samples did not differ from each other ($p < 0.05$). The values found for the low, medium, and high molecular weight films were 18.82 ± 0.03, 18.76 ± 0.44, and 18.50 ± 0.50, respectively. Based on the results, it is possible to observe that the molecular weight of chitosan influences the water solubility and water vapor permeability of the films, without influencing the moisture content. In conclusion, these findings suggest that the selection of chitosan molecular weight can tune the physicochemical properties of films for biodegradable packaging.

Agradecimentos/Acknowledgments

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Evaluation of the Cu(II) adsorption capacity of sodalite synthed from water treatment plant sludge

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Palavras Chave:*Cu(II) adsorption,Sodalite,Effluent Treatment,Zeolites,Porous Materials Chemistry*

Highlights

- Sodalite as adsorbent materials.
- Cu^{2+} adsorption onto porous sodalite.
- Structural and textural characterization.
- Evaluation of Cu^{2+} adsorption.

Resumo/Abstract

Sodalite is a zeolitic mineral to the feldspathoid group is classified as an aluminosilicate. Its crystalline structure consists of interconnected silicon (SiO_4) and aluminum (AlO_4) here tetrahedra, a rigid three-dimensional framework with internal cavities. These cavities mainly host sodium ions (Na^+) and anions, such as Cl^-, which ensure charge balance within the structure. Sodium plays a structural role and can be partially replaced by other cations, imparting ion-exchange capacity to sodalite. This property makes sodalite a promising material for environmental applications, in the removal of heavy metals such as copper. Sodalite zeolite synthesized from water treatment plant (WTP) sludge was supplied by Embrapa Instrumentation and obtained by a conventional hydrothermal method, followed by washing to pH 9 and drying at 100 °C.Sodalite was evaluated as adsorbents for Cu^{2+} removal. Adsorption experiments were carried out by contacting the materials with copper ion solutions in Falcon tubes (final volume of 10 mL), followed by incubation at 30 °C and 100 rpm for 24 h. After centrifugation, the supernatants were filtered, diluted to 250 µg L^{-1}, and analyzed by ICP-OES to determine the residual Cu^{2+} concentration and adsorption efficiency, demonstrating a Cu(II) adsorption capacity of up to approximately 50 mg g^{-1} for sodalite. After physicochemical characterization; the FTIR spectrum of sodalite exhibited a strong band centered at 965 cm^{-1} characteristic of Si–O and Al–O tetrahedral vibrations. XRD analysis showed no significant changes in the diffraction pattern after Cu^{2+} adsorption, indicating preservation of the crystalline structure. In contrast, BET analysis revealed an increase in surface area after copper adsorption.
Machado, R. C.; Valle, S. F.; Chao, I. R. S.; Ribeiro, C. Valorization of alum sludge waste through zeolite synthesis for sustainable fertilizer production. Materials Research, v.27, e20240269, 2024. DOI: 10.1590/1980-5373-MR-2024-0269

Agradecimentos/Acknowledgments

LAQSUPRA, PPGQ - CT, EMBRAPA INSTRUMENTAÇÃO, LAITEC, CEANMED.

Extração de melanina e queratina de cabelo humano utilizando solventes eutéticos profundos naturais (NADES) para potencial uso em biomateriais

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Palavras Chave:*Cabelo Humano,Queratina,Melanina,Solventes Eutéticos Profundos naturais,Reaproveitamento de Resíduos*

Highlights

NADES aplicados à extração sustentável de queratina e melanina de cabelo humano residual viabilizam biomateriais funcionais com potencial para engenharia de tecidos.

Resumo/Abstract

Mais de 300 mil toneladas de cabelo humano são descartadas anualmente em todo o mundo, sendo apenas uma pequena fração reaproveitada. Nesse contexto, este trabalho investiga uma abordagem sustentável para a extração de queratina e melanina a partir desse resíduo utilizando solventes eutéticos profundos naturais (NADES), visando à valorização de biomassa e ao desenvolvimento de biomateriais funcionais. A queratina é uma proteína estrutural com reconhecida biocompatibilidade e potencial aplicação em engenharia de tecidos, enquanto a melanina apresenta propriedades antioxidantes e semicondutoras, tornando-se atrativa como componente funcional em sistemas bioativos e potencialmente condutores. Diferentes formulações de NADES foram avaliadas. Para a extração de queratina, empregaram-se sistemas à base de cloreto de colina combinado com etanolamina, ácido oxálico e ácido fosfórico, além do NADES L-cisteína:ácido lático, que se destacou como promissor em função de sua capacidade de interagir com ligações dissulfeto e permitir a extração sob condições mais brandas. Para a extração de melanina, foram investigados diferentes sistemas, com destaque para o NADES cloreto de colina:ácido lático, selecionado devido à sua adequação à solubilização de biopolímeros aromáticos e à preservação de características estruturais associadas à condutividade. Os sistemas baseados em NADES foram comparados a métodos convencionais quanto ao rendimento e às propriedades físico-químicas dos biopolímeros obtidos. A queratina extraída está sendo aplicada na formulação de hidrogéis reticulados enzimaticamente, com posterior incorporação da melanina como fase funcional, visando conferir propriedades antioxidantes e potencial condutividade elétrica aos materiais. Os hidrogéis serão processados na forma de arcabouços tridimensionais por moldagem e impressão 3D e caracterizados quanto às propriedades estruturais, mecânicas, reológicas e elétricas, incluindo a avaliação da condutividade.

Agradecimentos/Acknowledgments

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Fertilizer-Dependent Performance of CNF/TPS-Based Controlled Release Devices

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Palavras Chave:*Enhanced Efficiency Fertilizer (EEF),Controlled release nutrient,Polymer processing,Sustainable agriculture*

Highlights

CNF/TPS-based devices were successfully developed as enhanced-release fertilizer systems, with fertilizer type significantly influencing processing behavior, morphology, and overall performance.

Resumo/Abstract

The study and development of enhanced efficiency fertilizers (EEF) are closely associated with contemporary socio-environmental challenges, such as population growth, the consequent increase in food demand, and the environmental impacts arising from the intensive use of conventional agricultural inputs, including groundwater contamination by microplastics. In this context, strategies based on biopolymeric materials have emerged as promising alternatives to improve nutrient and reduce environmental impacts. This study aims to standardize the formulation of EEF systems to evaluate the influence of different fertilizers sources on the physicochemical, structural, and performance properties of the materials. A comparative analysis was conducted on composites developed from monoammonium phosphate (MAP), magnesium sulfate ($MgSO_4$), and potassium nitrate (KNO_3), using cellulose nanofibrils (CNF) as an encapsulating agent. Microspheres containing each fertilizer (MsMAP, $MsMgSO_4$, and $MsKNO_3$) were produced by spray drying and subsequently incorporated into a thermoplastic starch (TPS) matrix through thermal processing. The materials exhibited distinct behaviors in terms of morphology, yield, and ionic release. Drying yields of 39.26 ± 0.26%, 44.14 ± 1.00%, and 52.33 ± 0.27% were obtained for MsMAP, $MsMgSO_4$, and $MsKNO_3$, respectively, indicating efficient encapsulation for KNO_3 and a more delayed release profile. Torque analysis revealed that salt nature strongly affects processing and rheological behavior, with KNO_3 exhibiting a pronounced plasticizing effect, resulting in lower maximum torque (16 Nm) and a monophasic morphology observed by SEM. Accelerated release tests in aqueous medium showed gradual release profiles for all systems, with superior performance observed for the TPS/$MsMgSO_4$ composite. Overall, the results demonstrate the feasibility of the CNF/TPS combination for developing EEFs with different salts and environmentally sustainable agricultural technologies.

Agradecimentos/Acknowledgments

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Fluorescent film applied to the adsorption and detection of glyphosate in water from Amazonian family farming

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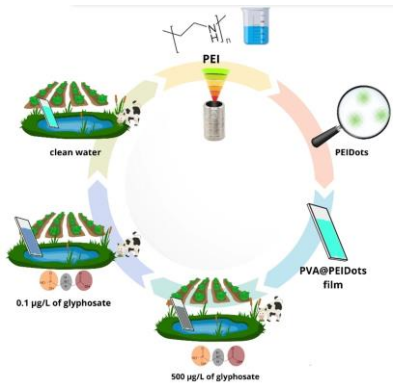
Palavras Chave:*Functional Photoluminescence,Adsorbent Nanoarchitecture,Active Biopolymers,AgroMonitoring,Adsorbent*

Highlights

Development of fluorescent films for detection and adsorption of herbicides in aquatic systems Advanced strategies for simultaneous removal and optical detection of agrochemical residues.

Resumo/Abstract

A intensificação da agricultura na região Amazônica tem exacerbado a contaminação hídrica por herbicidas persistentes, como o glifosato, demandando o desenvolvimento de tecnologias multifuncionais para monitoramento e remediação. Este trabalho apresenta a síntese e aplicação de um filme nanocompósito inovador, constituído por uma matriz de poli(álcool vinílico) (PVA) reticulada incorporada com pontos quânticos de carbono derivados de polietilenoimina (PEIDots). A caracterização estrutural via FTIR, Raman e microscopias (MEV/AFM) confirmou a dispersão homogênea das nanoestruturas e o aumento significativo da rugosidade superficial e energia de adesão, essenciais para a interação com o analito. O desempenho do compósito PVA@PEIDots destacou-se pela bifuncionalidade. Nos ensaios de remediação, o material exibiu cinética de adsorção rápida, atingindo o equilíbrio em 200 segundos, governada por um mecanismo de pseudo-segunda ordem. A capacidade máxima de adsorção (qe) alcançou cerca de 110 mg g^{-1} em pH 6,0, superando a matriz de PVA pura (95 mg g^{-1}), devido à introdução de sítios ativos nitrogenados e ao aumento do intumescimento (601%). O ponto de carga zero (4,33) favoreceu a atração eletrostática com o glifosato em pHs compatíveis com as águas amazônicas, dispensando ajustes químicos prévios. Simultaneamente, o filme demonstrou eficácia como sensor óptico. A presença de glifosato provocou a supressão sistemática (quenching) da fluorescência azul intensa dos PEIDots. Este fenômeno de quenching correlacionou-se à concentração do herbicida, permitindo a detecção qualitativa e quantitativa do contaminante na mesma plataforma utilizada para a remoção. Testes de estabilidade confirmaram a robustez do sinal fluorescente por 30 dias e a manutenção de 75% da capacidade adsortiva após 10 ciclos de reuso. Conclui-se que o PVA@PEIDots representa uma tecnologia promissora, sustentável e de baixo custo para o controle ambiental em áreas de agricultura familiar.



Synthesis of PVA@PEIDots film for glyphosate removal

Agradecimentos/Acknowledgments

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Fractional-Factorial Optimization of Graphene Oxide Thiolation Followed by Sulfonation

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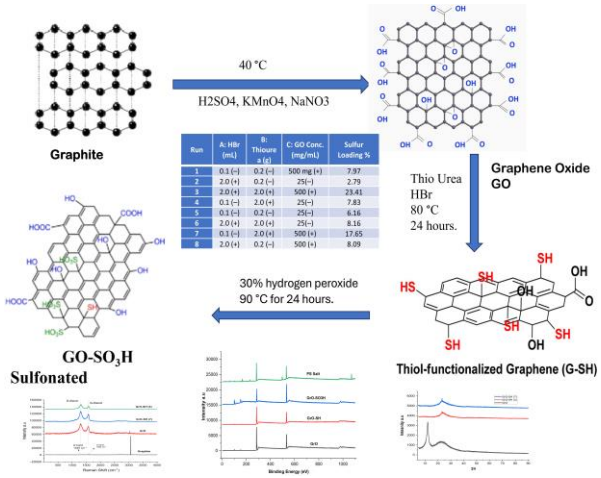
Palavras Chave:*Graphene oxide;,Acid Nanomaterials;,Thiolation,Sulfonation;,Design of Experiments (DoE)*

Highlights

A fractional factorial screening DoE significantly boosted Sulphur loading during GO thiolation.

Resumo/Abstract

Graphene oxide (GO) is a versatile two-dimensional platform whose properties can be engineered by controlled surface functionalization. Here, GO was synthesized from natural graphite via a modified Hummers oxidation and subsequently converted into thiol- and sulfonic acid-functionalised derivatives through a simple, scalable, wet-chemistry route. Thiolation was achieved by sequential treatment with hydrobromic acid (HBr) and thiourea (80 °C, 24 h), producing thiol-functionalised graphene (G–SH). A screening fractional factorial design of experiments was used to quantify the effects of GO loading, thiourea concentration, and HBr concentration on sulphur incorporation at constant temperature, enabling identification of significant main effects and interaction terms and guiding rapid optimization of the reaction window. Under the optimized conditions, highly thiolated materials were obtained, reaching sulphur contents as high as ~20–23% (depending on run conditions), which is substantially higher than typically reported for wet-chemical thiolation of GO. The thiolated material was then oxidatively converted into sulfonated graphene oxide (GO–SO_3H), introducing strongly acidic surface sites relevant to solid-acid catalysis and interfacial proton transport. Successful sequential functionalization (GO → G–SH → GO–SO_3H) was confirmed by complementary spectroscopy and microanalysis (FTIR, Raman, SEM–EDS, and XPS), including the emergence/shift of sulphur chemical states and characteristic vibrational signatures. Overall, this work establishes a tunable, design-guided strategy to access sulphur-rich graphene derivatives, with potential in catalysis, adsorption, electrochemical energy technologies, and membrane materials.



Pathway of Graphene oxide synthesis and thiol/sulfonic functionalization.

Agradecimentos/Acknowledgments

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From Dispersions to Thin Films: An SPM Study of MoS2 Flakes Decorated with AuNPs

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Palavras Chave:*Molybdenum Disulfide, Gold Nanoparticles, Thin Films, SPM, Nanocomposite*

Highlights

SPM analysis reveals a preferential decoration of AuNPs on the edges of the synthesized MoS_2 flakes, which causes a reduction in the work function of the AuNPs.

Resumo/Abstract

The properties of materials can be changed due to the synergistic effect of nanocomposites between 2D nanomaterials, such as molybdenum disulfide (MoS_2), and metallic nanoparticles, which can affect their properties. However, understanding the origin of these properties (such as morphology, roughness, friction, surface potential, deformation, adhesion, etc.) is important for the improvement of these nanomaterials.[1] In this work, dispersed samples and thin films of MoS_2 flakes decorated with gold nanoparticles (AuNPs) were characterized by Scanning Probe Microscopy (SPM) techniques. The nanocomposite was synthesized by the liquid-liquid interfacial route (LLIR)[2] using a water/toluene system, and, subsequently, the resulting film and dispersion were deposited in Si/SiO_2 substrates for analysis. Topographic image revealed that the edges of the synthesized MoS_2 flakes have spherical AuNPs anchored. Lateral Force Microscopy image confirmed the formation of the nanocomposite, where it shows a variation in friction between the MoS_2 flakes and the AuNPs. Furthermore, the samples were analyzed by Kelvin Probe Force Microscopy to map the surface potential and obtain the work function (WF) of the materials. The results in the dispersed sample indicate a good interaction between the two materials, where a reduction in the WF of the AuNPs occurred from 5.2 eV to approximately 4.9 eV. The average WF of the film varied between 4.8 and 5.1 eV, which may be related to greater agglomeration of the nanomaterials. These results show the versatility of SPM techniques in elucidating the properties arising from synergistic interactions between the materials.
[1] PEREIRA, Amanda F. et al.**Nanoscale**, 17 (16), p. 9974-9985, 2025.
[2] ZARBIN, Aldo J. G.**Materials Horizons**, 8 (5), p. 1409-1432, 2021.

Agradecimentos/Acknowledgments

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From MOF Architecture to Function: Sponge-like Copper–Gallic Acid Nano/Microspheres for Bio and Agro Applications

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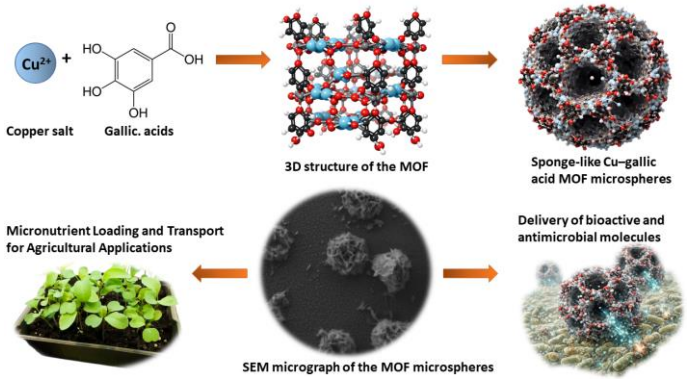
Palavras Chave:*Metal–organic frameworks (MOFs),Hierarchical porous materials,Green aqueous self-assembly,bioactive molecule delivery,sustainable agrochemicals*

Highlights

- Sponge-like Cu–gallic acid MOF microspheres
- Green aqueous Cu–polyphenol self-assembly
- Multiscale porous architecture confirmed
- Biocompatible antimicrobial agro-bio platform

Resumo/Abstract

Sponge-like microspheres based on a copper–gallic acid metal–organic framework (MOF) constitute a new hierarchical materials platform in which architecture governs function [1–3]. These highly porous structures, with sizes of approximately 1–2 µm, are formed via hydrothermal self-assembly through Cu–polyphenol coordination networks, generating an interconnected three-dimensional pore system. Scanning and transmission electron microscopy (SEM and TEM) reveal a highly porous, sponge-like morphology, while spectroscopic analyses (FTIR and solution-state NMR) confirm Cu^{2+}–ligand coordination and the preservation of phenolic groups. Powder X-ray diffraction (PXRD) evidences structural organization across multiple length scales, in agreement with the architecture observed by microscopy. Preliminary phytotoxicity assays performed with arugula (*Eruca sativa*), aimed at evaluating the compatibility of the material with plant systems and its potential agricultural application, indicate excellent biocompatibility at the applied concentrations. In parallel,*in vitro*biological studies are being conducted, including cytotoxicity evaluation by XTT assay and clonogenic assays, to assess the biological response and biosafety profile of the material. Complementary studies using AFM, SAXS, and BET analysis are planned to complete the multiscale characterization of the material. In addition, solution-state NMR studies in aqueous media will be performed to investigate the dynamics of water and bioactive molecules of interest confined within the porous framework. Antimicrobial assays are also being carried out to evaluate the intrinsic activity of the copper–gallic acid framework and its performance as a platform for the loading and release of bioactive molecules. Collectively, these studies support the ongoing development of this material for future agro- and bio-related applications. [1–3] Santoso et al. 2025; Elmehrath et al. 2024; Azhar et al. 2020



From molecular coordination to functional Cu–gallic acid MOF microsponges for agro-bio uses.

Agradecimentos/Acknowledgments

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From network structure to primary thermometry: Integrated characterization of RE3+-doped high-TeO2-content glasses

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Palavras Chave:*tellurite glass,luminescence thermometry,rare-earth ions,structure-properties relationship,upconversion*

Highlights

- RE^{3+}:TeO_2 structure-property link.
- Primary thermometry (100–550K).
- Er/Yb & Eu calibration-free sensing.
- Max sensitivity 1.1% K^{-1}.
- Robust next-gen photonic sensors.

Resumo/Abstract

Tellurite (TeO_2) glasses are exceptional hosts for photonic applications due to their high refractive indices and excellent rare-earth (RE^{3+}) solubility. This work provides a comprehensive investigation into the structure-property relationships and thermometric performance of RE^{3+}-doped pure TeO_2 glasses. Using advanced structural probes, including Raman spectroscopy, solid-state NMR, and EPR, we elucidate how dopants such as Eu^{3+}, Sc^{3+}, and Yb^{3+} are accommodated within the tellurite framework, specifically identifying the formation of non-bridging oxygens and network rearrangements. Building on this structural foundation, we characterize the glasses' potential for calibration-free luminescence thermometry using both emission- and excitation-based approaches. Er^{3+}/Yb^{3+} co-doped samples demonstrated reliable primary thermometry between 250-550 K via upconversion from thermally coupled levels, yielding a relative sensitivity (SR) of 1.1% K^{-1} at 300 K. Additionally, Eu^{3+} excitation-based thermometry exhibited high experimental-modeled agreement across the 100-520 K range (SR approx 0.5% K^{-1}). Our findings establish high-TeO2-content glasses as robust, versatile platforms for next-generation optical temperature sensing, linking intrinsic structural flexibility to high-performance thermometric operation.

Agradecimentos/Acknowledgments

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Functionalization of Cellulose Nanofibrils: Comparative Ecotoxicity Assessment Using the Zebrafish Model

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Palavras Chave:*Nanocellulose,Nanosafety,Cellulose nanofibrils,Surface charge,Zebrafish embryos*

Highlights

- Toxicity screening of functionalized nanocelluloses.
- Surface charge influence on toxicity to zebrafish embryos.
- Developmental delays caused by cationic nanocellulose.

Resumo/Abstract

Nanocelluloses have emerged as prominent green materials in nanotechnology and materials science, finding applications in diverse fields such as sensors, water decontamination, and electronics. These applications leverage their unique properties, including renewability, abundance, high mechanical strength, biocompatibility, and chemical stability. To enhance their physicochemical properties and functional potential, various surface modifications are employed, such as TEMPO-mediated oxidation and cationization. Despite being frequently characterized as safe, some studies have reported adverse effects associated with nanocellulose exposure, including inflammatory responses, genotoxicity, and oxidative stress. Consequently, toxicity screening using zebrafish (*Danio rerio*) embryos has become advantageous due to the model's low cost, ease of maintenance, and genetic similarity to mammals, establishing it as a robust alternative in toxicological research. In the present study, two types of cellulose nanofibrils were synthesized: anionic nanofibrils via TEMPO oxidation (aCNF) and cationic nanofibrils through quaternary ammonium functionalization (cCNF). The resulting materials were characterized using TEM, AFM, zeta potential, and FT-IR. Toxicity assays conducted with zebrafish embryos revealed an LC_{50} of 12.55 (9.89–15.5) mg/L for cCNF, whereas no lethal effects were observed for aCNF up to 73 mg/L. Additionally, cCNF exposure caused developmental delays in the larvae, a phenomenon not detected in the aCNF groups. These findings demonstrate that different surface charges result in distinct toxicological profiles, highlighting the necessity of safety assessments when selecting functionalization pathways for nanomaterials, aiming Safe-by-Design approaches for safer materials.

Agradecimentos/Acknowledgments

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GEOPOLYMERS: PRECURSOR SYNTHESIS AND WASTE ADDITION FOR APPLICATION IN CIVIL CONSTRUCTION

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Palavras Chave:*Geopolymer,sodium silicate,metakaolin,waste reuse,sustainable civil construction*

Highlights

Sodium silicate produced from residual sand. Reactive metakaolin obtained by optimized calcination. Mining residues used as additives in geopolymers.

Resumo/Abstract

Geopolymers are a sustainable option for the civil construction sector due to their structural and environmental advantages, especially the reduction in carbon dioxide emissions compared to conventional concretes, which contributes to Sustainable Development Goal (SDG) 13, aimed at improving the global climate. However, the high cost of raw materials still limits their application. This study aimed to develop a route for the synthesis of precursors and geopolymer formulations incorporating mining waste in order to reduce production costs.

To produce the sodium silicate precursor, 32.6% residual sand, 54.3% analytical-grade solid sodium hydroxide, and 13.0% deionized water were mixed (Na_2O/SiO_2 molar ratio close to 2.5). The mixture was treated at 450 °C for 100 minutes, resulting in a solid material. The chemical analysis of the product was performed by acid–base titration. The metakaolin precursor was obtained by calcination of kaolin in an industrial furnace at 700 °C for two hours and characterized by X-ray diffraction. Samples of slag, silica fume, and mining wastes from lithium and rare-earth extraction were collected and ground for use as additives.

Subsequently, several geopolymer formulations were prepared in the laboratory, in which the precursors, additives, and water were mixed and manually molded to produce test specimens for compressive strength testing after curing periods of 1, 3, and 7 days. The results were analyzed in accordance with NBR 9781:2013, and the most satisfactory composition, which reached a compressive strength of 47 MPa at 7 days, was 34.1% metakaolin, 17.13% sodium silicate, 19% slag, and 29.7% water (values shown in Table 1). These results indicate that the material can be applied in the production of interlocking paving blocks and coatings. The next step is to evaluate geopolymer production on a larger scale to validate a production chain with lower cost and reduced environmental impact for the civil construction sector.

Table 1.

Curing time (in days)	Strength (in MPa)
1	20.71
3	41.34
7	46.94

Results of compressive strength (MPa) of samples after 1, 3 and 7 days of curing.

Agradecimentos/Acknowledgments

The authors thank FAPEMIG, ESCALAB, and the Department of Chemistry at UFMG for the financial and institutional support for the execution of this project.

Glycerol-based coordination compounds as a strategic precursor of electrode materials for energy storage

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Palavras Chave:*Coordination compound, Lithium-ion batteries, Sodium-ion batteries, Layered transition metal oxide, Energy storage*

Highlights

Layered NCM111 and NFM111 cathodes synthesized from metal-glycerolates deliver ~130 mAh g^{-1}, highlighting a sustainable route for LIBs and SIBs.

Resumo/Abstract

Glycerol has been reported as a highly promising molecule in the design of a wide range of nano- and micromaterials for strategic applications in the energy transition. Among the various uses of glycerol in chemical syntheses, the development of synthetic routes to prepare metal-glycerolates (M-Glys) has emerged as a particularly innovative approach, both for direct application and as precursors to active electrode materials. In this work, the design of different cathode active materials for lithium-ion (LIBs) and sodium-ion batteries (SIBs) is presented, employing M-Glys as precursors synthesized by the solvothermal method. More specifically, layered transition metal oxide cathodes for LIBs and SIBs were prepared with compositions $LiNi_1/_3Co_1/_3Mn_1/_3O_2$ (NCM111) and $NaNi_1/_3Fe_1/_3Mn_1/_3O_2$(NFM111), respectively. As expected, the X-ray diffraction patterns of both NCM111- and NFM111-based cathode materials reveal O3-type layered structures. In both cases, scanning electron microscopy images reveal microspheres composed of polyhedral primary particles. Additionally, preliminary results show a specific capacity of 129 mAh g^{-1} for NCM111, whereas for NFM111 it is approximately 130 mAh g^{-1} at 0.1C. Overall, these results demonstrate the viability of M-Glys as versatile and effective precursors for layered transition-metal oxide-based cathode active materials of LIBs and SIBs. This strategy opens new opportunities for rational materials design toward high-performance and sustainable energy storage systems.

Agradecimentos/Acknowledgments

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Gold nanorods coated with a porous Au–Ag alloy as resonant plasmonic structures for active SERS platforms via the self-assembled monolayer method.

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Palavras Chave:*Surface-Enhanced Raman Scattering (SERS),Gold nanorods,Au@Ag core–shell nanostructures,Self-assembled monolayer (SAM),Rhodamine 6G*

Highlights

Au and Au@Ag core–shell nanorods were assembled via SAM optimization and evaluated as plasmonic SERS platforms for rhodamine 6G detection.

Resumo/Abstract

Raman spectroscopy has been widely explored as an analytical technique for applications ranging from environmental monitoring to biomedical analysis. However, its practical implementation is often limited by the inherently weak Raman scattering cross section, particularly at trace analyte concentrations. To overcome this limitation, surface-enhanced Raman scattering (SERS) has emerged as an effective strategy to increase signal intensity by exploiting the plasmonic response of metallic nanostructures. In this work, gold nanorods (AuNRs) were synthesized and further engineered through sequential surface modification steps, including silver shell deposition (Au@AgNRs) followed by a galvanic replacement process using $AuCl_4^-$, resulting in nanorods coated with a porous Au–Ag alloy shell (Au@hAuAgNRs). The optical properties of the nanostructures were investigated by UV–Vis spectroscopy, revealing localized surface plasmon resonance (LSPR) bands at 525 and 759 nm for AuNRs, 504 and 665 nm for Au@AgNRs, and 521 and 760 nm for Au@hAuAgNRs. These spectral features are consistent with transverse and longitudinal plasmon modes and confirm the successful structural evolution at each synthesis stage. The nanostructures were integrated into SERS platforms by immobilization onto silicon substrates functionalized with 3-mercaptopropyltrimethoxysilane. Nanoparticle adsorption was optimized using a self-assembled monolayer (SAM) approach with immersion times of 24, 48 and 72 h. SERS performance was evaluated using rhodamine 6G (R6G, 10^{-3} mol.L^{-1}) as a probe molecule. Preliminary results indicate that immersion times of 48 h and 72 h provide enhanced Raman signals, yielding intensities of 49,195.5 and 34,073.8 counts, respectively. Ongoing studies will focus on a systematic comparison of Au@AgNRs and Au@hAuAgNRs based substrates under identical assembly conditions, as well as on reducing the analyte concentration to assess the detection sensitivity of the developed SERS platforms.

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Graphite Inks for Green Printed Electronics

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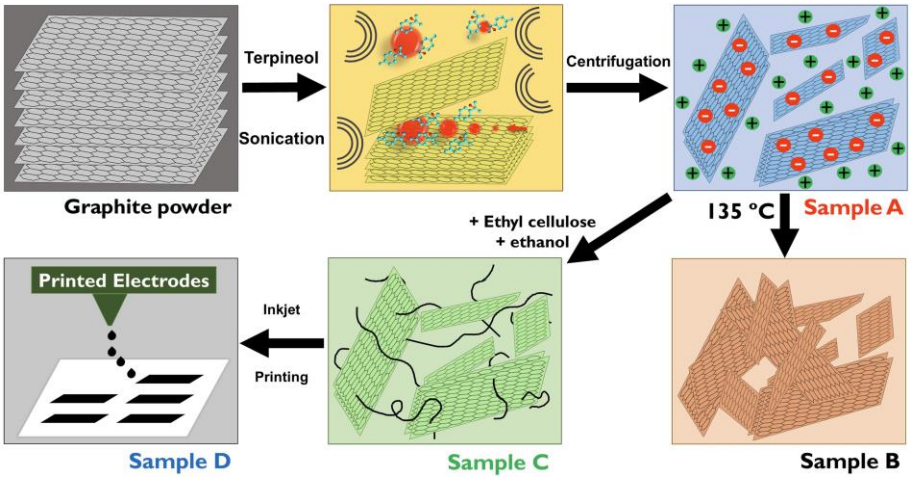
Palavras Chave:*Carbon materials,Asphaltenes,Organic Electronics,Green Electronics,Conductive Inks*

Highlights

Conductive graphtite inks composed only of environmentally friendly and renewable additives were inkjet-printed on paper resulting in flexible electrodes.

Resumo/Abstract

Liquid-phase exfoliation of graphite was conducted using terpineol as exfoliating agent for the first time in the literature and the resultant dispersion was formulated into conductive and inkjet-printable inks composed only of environmentally friendly and renewable additives. Graphite exfoliation was probed and confirmed that terpineol is a mild exfoliating agent and a viable alternative to toxic and non-renewable solvents. The graphite dispersion presents particles with nanoplatelets morphology, lateral sizes between 500 and 900 nm and mean size of 700 nm, mass concentration of 3.8±0.2 mg mL^{-1}, shelf life of 3 years and 51 days considering a 1 mm sedimentation, and the calculated energy barrier for the coagulation is 53×kBT. Such very high shelf life and colloidal stability were never reported for a graphite-based organic dispersion and are consequences of the electrostatic repulsion between the dispersed nanoplatelets in terpineol, which acquire electrical charges during sonication and present a mean zeta potential of −72 mV estimated from a homocoagulation experiment. The green conductive formulations were prepared using less steps than similar reports and exhibit good printability and maintain the colloidal stability during many hours of printing, which are great achievements concerning carbon-based inks. Electrodes printed on paper using two different inks resulted in Ohmic devices, and sheet resistances of 4.36±0.51 and 0.94±0.03 kΩ sq^{-1} were obtained printing 10 and 30 layers of the best formulation, respectively. The results confirm the exfoliating and stabilizing capabilities of terpineol and the remarkable printing performance of the green formulations, paving the way for novel developments in Green Electronics.



Scheme of the samples' preparation.

Agradecimentos/Acknowledgments

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H2 adsorption and dissociation in Pd clusters and surfaces

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Palavras Chave:*Pd clusters and surface, H2 absorption and dissociation, DFT calculations*

Highlights

The H_2 absorption and dissociation in Pd systems allow us to assess the availability of H species, for example, for subsequent CO_2 hydrogenation.

Resumo/Abstract

We performed DFT calculations with Gaussian for Pd_1–Pd_6 clusters using the M06 functional hybrid meta-GGA functional. For a periodic Pd(111) slab, we used the CP2K package, with PBE generalized gradient approximation (GGA), GTH pseudopotentials, and MOLOPT triple-ζ basis sets, including D3 dispersion corrections.Initial adsorption configurations were constructed using five Pd(111) adsorption sites: on-top (**T**), bridge 1 ($\mathbf{B}_1$) and 2 ($\mathbf{B}_2$), and hollow - FCC (**H**FCC)/HCP (**H**HCP). H_2 adsorption and dissociation were studied in both periodic (**Table 1**) and finite (**Table 2**) models (clusters) to identify the most favorable cluster geometries and adsorption sites for H–H bond activation, as quantified by the stretched H−H distance and the weakened bond, as well as adsorption energies and dissociation barriers. For the molecular calculations (clusters), transition states were given by TS optimizations. For the periodic Pd(111) slab, minimum-energy paths will be obtained using the nudged elastic band (NEB) method, enabling consistent assessment of transition states and reaction barriers across the two descriptions and allowing us to evaluate the availability of H species for subsequent CO_2 hydrogenation. The def2-TZVP basis set (Triple-Zeta Valence with Polarization) was employed. The M06 functional (Minnesota functional) is classified as a hybrid meta-GGA functional.

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Table 1. Four lowest-ΔE structures out of 15 initial adsorption configurations of H_2 on Pd(111) in the periodic system. The H_2 molecular orientation (X, Y, or Z). Adsorption energies (E_{ads}), ΔE is the relative energy (kJ / mol) with respect to the lowest-energy structure among the calculated configurations and d_{H-H} is the optimized H–H distance.

H_2 orientation	Site	E_{ads} (kJ / mol)	ΔE (kJ / mol)	d_{H-H} (Å)
Y	*T*	-69.88	0.00	0.84
X	*T*	-69.44	0.44	0.84
Y	B_2	-69.76	1.26	0.84
Z	*T*	-52.67	17.21	0.77

Table 2. The lowers adsorption energies (E_{ads}), transition-state energies (TS) relative to the adsorption state, and relative energy (ΔE) for H_2 on Pd clusters Pd_n (n = 1–6), obtained from molecular calculations.

System	E_{ads} (kJ / mol)	ΔE (kJ / mol)	d_{H-H} (Å)	TS (kJ / mol)
Pd + H_2	-76.19	117.79	0.845	123.81
Pd_2 + H_2	-186.42	7.56	1.981	249.08
Pd_3 + H_2	-193.98	0.00	2.224	18.57
Pd_4 + H_2	-152.98	41.00	2.355	0.67
Pd_5 + H_2	-43.78	150.02	2.121	7.48
Pd_6 + H_2	-112.34	81.64	3.437	39.42

Tables

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Hybrid Graphene/CuxO/Ag Nanostructures as Thin and Transparent Platforms for Surface-Enhanced Raman Scattering

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Palavras Chave:*Surface-Enhanced Raman Scattering (SERS), Plasmonic Nanoparticles, Transparent Thin Films, Hybrid Nanocomposites*

Highlights

- One-step interfacial synthesis yields thin and transparent rGO/Cu_xO/Ag hybrid films with controlled composition and morphology for advanced SERS applications;

Resumo/Abstract

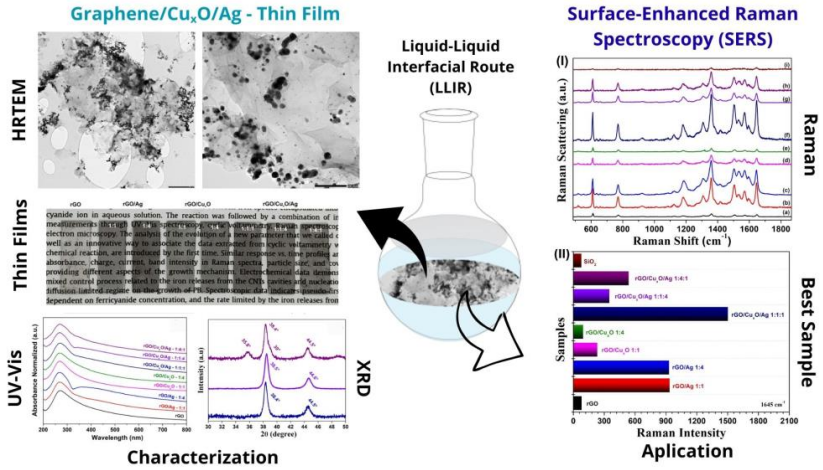
Surface-enhanced Raman spectroscopy (SERS) stands out as an ultrasensitive analytical technique capable of delivering molecular fingerprint information in a rapid, direct, and non-destructive fashion.[1] Yet, its ultimate performance is governed by the architecture and composition of the supporting substrate.[2] Here, we present the design and investigation of thin and transparent hybrid nanocomposite films based on reduced graphene oxide (rGO) decorated with copper oxide (Cu_xO) and silver nanoparticles, engineered as high-performance SERS substrates. The nanocomposites were synthesized in situ in a single step through a liquid–liquid interfacial route (LLIR-GQM)[3] using a two-phase system composed of water and toluene, with $AgNO_3$, $Cu(NO_3)_2$, graphene oxide, and $NaBH_4$. Fine control over precursor ratios enabled the fabrication of rGO/Ag, rGO/Cu_xO, and ternary rGO/Cu_xO/Ag films with tailored compositions. Spectroscopic analyses confirmed the coexistence of rGO and plasmonic silver, while X-ray diffraction identified crystalline phases of metallic silver and copper oxides. Electron microscopy revealed morphology strongly dictated by composition, with the emergence of hotspot-rich nanostructures in the ternary systems. SERS activity was assessed using rhodamine 6G as a molecular probe, revealing the rGO/Cu_xO/Ag (1:1:1) film as the most efficient substrate, delivering a sensitivity 10^4 times higher than SiO_2 and at least one order of magnitude above the other nanocomposites. These findings highlight the powerful synergy between graphene, silver, and copper oxide, positioning Cu_xO as a cost-effective and promising component for next-generation SERS platforms.

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Characterization of graphene/CuxO/Ag thin films and their application as SERS substrates.

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Hybrid Hexacyanoferrate-Based Filaments for the Fabrication of 3D Electrodes by Fused Filament Fabrication Applied to Energy Storage

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Palavras Chave:*Hybrid filaments,Hexacyanoferrates,Fused Filament Fabrication (FFF),Energy storage devices,3D printed electrodes*

Highlights

Prussian blue and niobium oxide were integrated into hybrid filaments for FFF printing of funcional 3D electrodes and enable 3D for energy storage applications. FFF enables controlled deposition 3D.

Resumo/Abstract

Prussian Blue (iron hexacyanoferrate, FeHCF) is a widely studied coordination compound characterized by its cubic open-framework structure, in which Fe^{2+} and Fe^{3+} ions are bridged by cyanide ligands. This three-dimensional lattice forms well-defined channels and interstitial sites, which facilitate rapid and reversible ion insertion and diffusion. Such structural features make FeHCF an attractive active material for electrochemical energy storage devices, including batteries and supercapacitors. Beyond its structural advantages, FeHCF exhibits high thermal and chemical stability, low cost, and environmental friendliness, enhancing its potential for scalable energy storage applications. Its electrochemical performance can be further enhanced by combining with niobium oxide (Nb_2O_5) and conductive carbon-based additives (rGO, carbon black), which improve electron transport and mechanical integrity. The integration of these components into hybrid filaments enables the fabrication of 3D electrodes with controlled architecture, expanding the versatility and efficiency of additive manufacturing for energy storage devices. The hybrid architecture integrates FeHCF/Nb_2O_5 synthesized via coprecipitation with carbon additives in solvent, ensuring homogeneous dispersion and efficient percolative networks. Characterizations (XRD, SEM, TEM, AFM, Raman, BET) confirmed thermal stability, high surface area, and structural integration. The 3D-printed electrodes demonstrated competitive aqueous electrochemical performance, achieving a specific capacity of 17.52 mAh g^{-1}, remarkable considering that only 10% of the electrode mass is active material and 65% is insulating PLA. The device retained 93–94% capacity after 200 cycles without surface post-treatments. Low-cost precursors, high reproducibility, and a biodegradable matrix highlight the scalability of this approach, establishing the hybrid filament as a versatile platform for customized energy storage devices.

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Hybrid nanoplatform based on graphene oxide, gold nanoparticles and porphyrin for photodynamic cancer therapy

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Palavras Chave:*Photodynamic therapy; Graphene oxide; Gold nanoparticles; Porphyrin; Nanohybrids*

Highlights

Hybrid GO–AuNP–porphyrin system for PDT

Synergistic plasmonic and photodynamic effects

Enhanced ROS generation under visible light

Comprehensive spectroscopic and microscopic characterization

Resumo/Abstract

Photodynamic therapy (PDT) is a minimally invasive strategy for cancer treatment based on the light activation of photosensitizers to generate reactive oxygen species (ROS). In this work, a hybrid nanoplatform composed of graphene oxide (GO), gold nanoparticles (AuNPs), and porphyrin molecules is investigated as a promising photosensitizing system for PDT applications.

Graphene oxide acts as a versatile two-dimensional support, providing high surface area and functional groups for the anchoring of AuNPs and porphyrins, while gold nanoparticles contribute plasmonic enhancement effects that can improve light absorption and ROS generation. Porphyrins, well-known photosensitizers, are incorporated to promote efficient singlet oxygen production upon visible light irradiation.

The hybrid materials are characterized using Fourier-transform infrared spectroscopy (FTIR), UV–Vis spectroscopy, electron paramagnetic resonance (EPR), and Raman spectroscopy to investigate chemical interactions, optical properties, and ROS generation mechanisms. Morphological and structural analyses are performed by transmission electron microscopy (TEM) and scanning electron microscopy (SEM), confirming the successful assembly of the nanocomposite.

The results to demonstrate synergistic effects between GO, AuNPs, and porphyrins, leading to enhanced photodynamic efficiency compared to isolated components. This study contributes to the development of advanced nanostructured photosensitizers and highlights the potential of graphene-based hybrid systems for cancer photodynamic therapy.

Agradecimentos/Acknowledgments

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Influência da morfologia das nanopartículas de Ag em associações Ag/Nb2O5 na fotodegradação de diclofenaco monitorada por fluorescência.

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Palavras Chave:*Fotocatálise,Degradação,Morfologia,Diclofenaco,Fluorescência*

Highlights

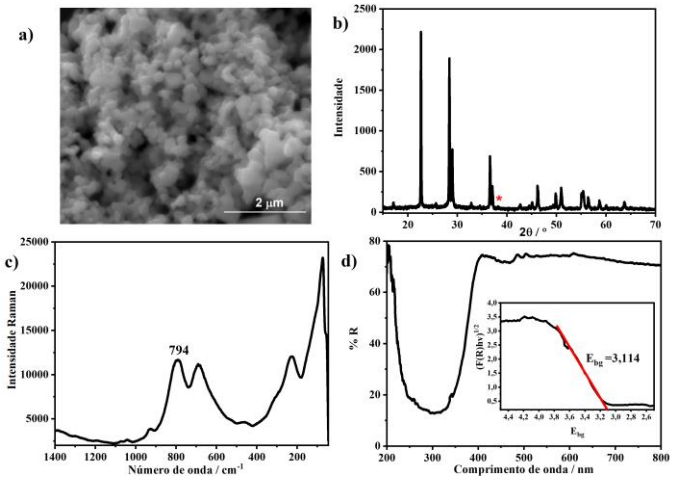
Hybrid Ag/Nb_2O_5 materials were synthesized and characterized. Silver addition reduced the semiconductor band gap and resulted in high diclofenac photodegradation performance.

Resumo/Abstract

O Brasil encontra-se entre os maiores consumidores de medicamento do mundo, ao mesmo tempo em que enfrenta deficiências significativas no saneamento básico. Em virtude desses fatores, estudos já evidenciaram a presença de fármacos como o diclofenaco em diferentes matrizes aquáticas, o que representa riscos tanto para o meio ambiente quanto para a saúde pública. Diante disso, este trabalho teve como objetivo a síntese, caracterização e avaliação da atividade fotocatalítica de materiais híbridos à base de Nb_2O_5 e nanopartículas de Ag com morfologia de esferas (AgNPs) e fios (AgNFs), visando à degradação do diclofenaco sob irradiação no visível.

Os catalisadores foram obtidos pela associação de AgNPs ou AgNFs ao Nb_2O_5, utilizando diferentes proporções Nb_2O_5:Ag. As soluções foram submetidas à sonicação e ao aquecimento a 60 °C por 1 h, seguidas de secagem para obtenção dos sólidos. A avaliação fotocatalítica foi realizada com solução de diclofenaco de sódio ($1{,}0\times10^{-5}$ mol L^{-1}), adicionando-se 50 mg do catalisador, com etapa prévia de adsorção por 24 h e monitoramento da degradação utilizando lâmpada de 150 W por 7 h via espectroscopia de fluorescência.

As técnicas de DRX, espectroscopia Raman, reflectância difusa no UV-VIS e MEV (Figura 1) confirmaram a presença dos componentes Nb_2O_5 e Ag nos sistemas híbridos. Os resultados de reflectância indicaram redução do*band gap*para determinadas proporções Nb_2O_5:Ag em comparação ao Nb_2O_5 puro, sugerindo potencial melhoria no desempenho fotocatalítico. Os espectros Raman revelaram modificações nos sistemas contendo a presença AgNPs, dada a intensificação e deslocamento da banda presente em 817 cm^{-1} no espectro do Nb_2O_5 puro. Por fim, os ensaios de fotodegradação do diclofenaco apresentaram desempenho superior ao Nb_2O_5 puro na degradação do fármaco sob irradiação visível, indicando ganho significativo na taxa de degradação.



Análise do catalisador 80Nb2O5:20AgNP: a) MEV; b) DRX; c) Espectro Raman; d) Reflectância difusa.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG, UFJF

Influence of Aromatic Substituents in Aniline Derivatives on the Formation of Low-dimensional Lead Halide Hybrid Perovskites

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Palavras Chave:*Hybrid lead halide perovskites; Ruddlesden–Popper perovskites; Aromatic organic spacers; Amine basicity modulation; Perovskitoids.*

Highlights

Aniline acts as an aromatic spacer forming water-stable perovskitoids. Electrophilic aromatic substitution modulates amino basicity. Synthesis of perovskites with modified aniline.

Resumo/Abstract

Due to the possibility of tuning their optical and electronic properties, together with the feasibility of synthesis through relatively simple chemical routes, hybrid lead halide perovskites have become materials of great relevance for optoelectronic applications. In this context, low-dimensional perovskites, particularly those belonging to the Ruddlesden–Popper (RP) family, have attracted increasing attention owing to the enhanced structural stability provided by the intercalation of hydrophobic organic spacers between the inorganic layers. Among the various organic spacers, aniline stands out due to its aromatic character and its ability to significantly influence the structural organization of the material, leading to the formation of water-stable lead halide perovskitoids with stoichiometry $(A)_3Pb_2Br_7$.

Aiming to deepen the understanding of the mechanisms governing the formation of these structures, this work systematically investigates the chemical modification of the aniline molecule by introducing electron-donating and electron-withdrawing substituents onto the aromatic ring. The main objective is to modulate the basicity of the amino group and to evaluate the direct impact of these molecular modifications, including electronic and steric effects, on the structural formation of the hybrid materials, assessing whether such variations favor the formation of RP-type phases or preferentially lead to the formation of perovskitoids.

The synthesis, purity, and structure of the obtained molecules were confirmed by Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and melting point analysis. The hybrid lead halide perovskites derived from these molecules were characterized by X-ray Diffraction (XRD) for crystalline phase identification, and their morphology was investigated using scanning electron microscopy (SEM).

Agradecimentos/Acknowledgments

The authors acknowledge the financial support from FAPESP (grants no. 2024/15260-2, 2023/12165-6 and 2022/06433-5) and the UFABC experimental multiuser center (CEMUFABC).

Influence of Temperature on the Morphological Modification of Nb_2O_5 Nanostructures

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Palavras Chave:*: Niobium Pentoxide (Nb_2O_5),Hydrothermal Synthesis,Nanostructures,Morphology*

Highlights

Nb_2O_5 nanostructures were hydrothermally synthesized (120–160 °C); higher temperatures induced phase and morphology changes, affecting surface area and porosity.

Resumo/Abstract

Niobium is a transition metal that has attracted significant scientific and industrial interest due to its properties, such as high thermal stability, corrosion resistance, and relevant chemical and physical characteristics, especially for catalytic applications. This interest arises from the ability of its different crystalline phases to tune properties such as surface area and the number of available acidic sites. In nature, niobium is predominantly found as oxides, with niobium pentoxide (Nb_2O_5) being the most stable form, exhibiting several polymorphic phases.[1–3] In this work, Nb_2O_5 nanostructures were synthesized via an alkaline hydrothermal route to investigate the influence of temperature on the morphology and physicochemical and structural properties of the material. For the synthesis, 3 g of Nb_2O_5 were dispersed in 100 mL of NaOH solution (9 mol/L) and treated in a Teflon-lined reactor at different temperatures (120 - 160 °C) for 24 h. After synthesis, the materials were washed with 0.1 mol/L HCl solution until pH < 3.0 and subsequently with deionized water until pH 7.0. The samples were characterized by Scanning and Transmission Electron Microscopy (SEM and TEM), X-ray Diffraction (XRD), and specific surface area analysis using the BET method. SEM and TEM analyses showed that the synthesis temperature directly influences the morphology of the Nb_2O_5 nanostructures (Figure 1). The precursor material exhibited an amorphous character with a high degree of agglomeration. At 120 °C, greater dispersion of the nanostructures was observed, while at 130 °C more homogeneous nanowires were formed. At 140 °C, the coexistence of nanowires and microcubes was observed, whereas samples synthesized at 150 and 160 °C were predominantly composed of microcubes. XRD results confirmed the transition from an amorphous to a highly crystalline phase with increasing temperature, with predominance of the trigonal phase at 140 and 160 °C, in agreement with ICSD card No. 5408.[3,4] BET analysis indicated a decrease in specific surface area with increasing temperature, reaching the lowest values at 150 °C, followed by a slight increase at 160 °C. These results demonstrate that the hydrothermal route and temperature variation are effective strategies for structural modulation of niobium pentoxide.

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4. ICSD – Inorganic Crystal Structure Database. Entry No. 5308,*$NaNbO_3$.*

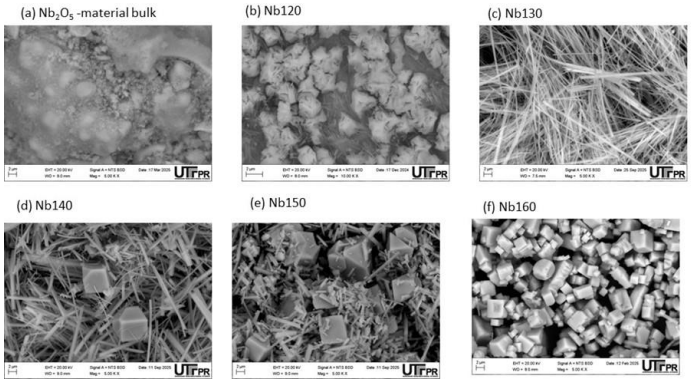


Fig. 1 – SEM image of the Nb_2O_5 nanostructure

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Influence of the Dissolution Method on Two-Step All-Cellulose Composites

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Palavras Chave:*Biopolymer,Carbon dioxide,Composite,Fiber-matrix interface,Film casting*

Highlights

Comparison of different cellulose solvent systems reveals distinct effects on chain degradation and fiber morphology in two-step all-cellulose composites.

Resumo/Abstract

The development of all-cellulose composites (ACCs) has gained increasing attention due to their potential as fully bio-based materials with competitive mechanical performance. Among the available processing routes, the two-step method stands out as a versatile approach, in which part of the cellulose is selectively dissolved to form a matrix phase while the remaining fibers act as reinforcement. In this context, the dissolution method plays a key role, since it may affect both the chemical integrity of the cellulose chains and the morphology of the reinforcing fibers, ultimately influencing the properties of the resulting composites. In this work, ACCs were produced in order to investigate the influence of the cellulose dissolution process. Two systems were evaluated, the conventional viscose process and the DMSO/DBU/CO_2 switchable solvent system. Viscosity measurements were performed to estimate changes in the degree of polymerization of the matrix after each treatment. The initial degree of polymerization of the cellulose pulp was 630. After dissolution, the DMSO/DBU/CO_2 system resulted in a value of 496, while the viscose process led to a lower value of 417, indicating a more pronounced degradation of the cellulose chains in the viscose route. However, scanning electron microscopy images revealed differences in the morphology of the reinforcing fibers after dissolution. The viscose-treated samples showed better preservation of the fibrous structure, whereas the DMSO/DBU/CO_2 system caused more noticeable structural alteration of the cellulose fibers. These results indicate that the two dissolution methods affect the chemical and morphological aspects of cellulose in different ways. Mechanical tests will be carried out as the next step to evaluate how these differences influence the performance of the resulting ACCs.

Agradecimentos/Acknowledgments

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Inkjet-Printed Au/Ag Nanoprism SERS Substrates for Discriminating Structurally Related Dyes

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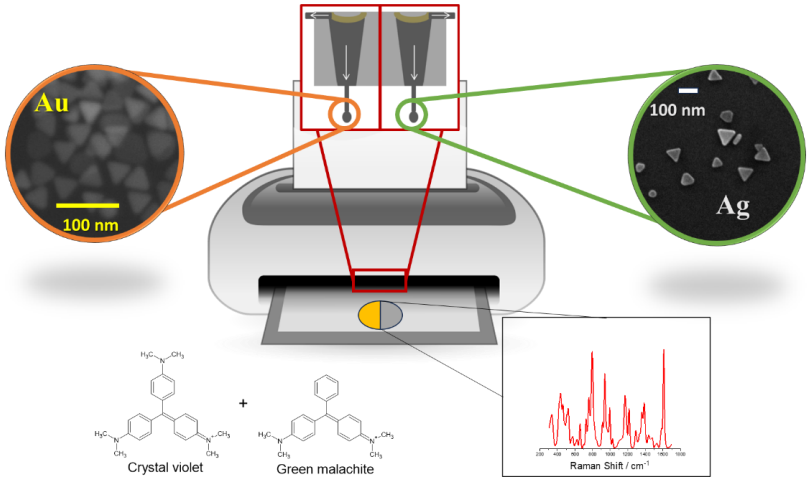
Palavras Chave:*SERS, inkjet printing, nanoprisms, molecular discrimination, plasmonics*

Highlights

Printed Au/Ag nanoprism substrates enable reproducible, composition-dependent SERS fingerprints for distinguishing similar dyes.

Resumo/Abstract

Inkjet printing offers a scalable route for producing portable and reproducible SERS substrates capable of reducing detection limits and analysis time. In this work, gold and silver triangular nanoprisms (AuTNPs and AgTNPs) were synthesized, formulated into stable inks, and printed side by side onto hydrophobized chromatography paper to evaluate how nanoparticle composition influences the SERS response of structurally related dyes, crystal violet (CV) and malachite green (MG). Electron microscopy and optical characterization confirmed that the nanoprism morphology was preserved after printing, with AuTNP-based substrates exhibiting superior spectral reproducibility and storage stability. The SERS spectra of CV and MG displayed clear composition-dependent vibrational fingerprints: AuTNPs provided higher enhancement factors and induced systematic band shifts and relative intensity variations that improved molecular discrimination. Artificial neural networks applied to CV/MG mixtures achieved mean prediction errors of 0.06 (training) and 0.11 (validation), with larger deviations associated with regions of lower enhancement. Overall, these results demonstrate that nanoprism composition plays a critical role in shaping SERS spectral features and that combining signals from distinct plasmonic nanostructures on printed paper substrates enhances both discrimination and quantitative analysis of closely related molecular species.



Nanoprisma de Au/Ag impressos por inkjet ajustam assinaturas SERS e melhoram a discriminação CV/MG

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP (2022/02893-1, 2023/06463-4) and CNPq (306073/2024-2, 444106/2024-3), and thank LNNano-CNPEM and LISpec (RRID: SCR_027391/CEMUIQ-UNICAMP) for technical support.

Insights into core-level excitations in non-fullerene acceptors

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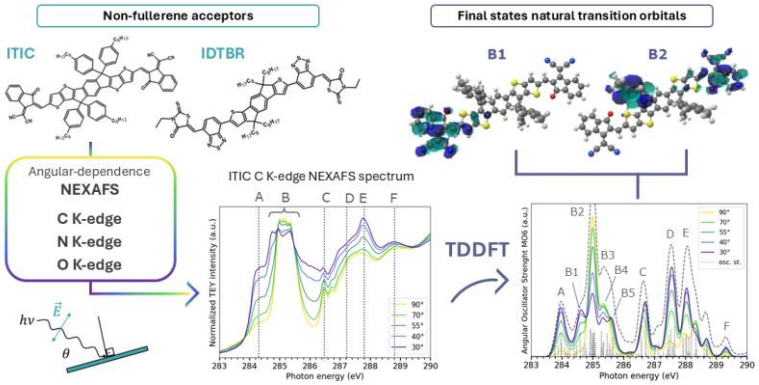
Palavras Chave:*NEXAFS,TDDFT,non-fullerene acceptors,small molecules,organic semiconductors*

Highlights

NEXAFS reveals complementary information among edges
Angular dependence allows molecular orientation and final state symmetry analysis
TDDFT angular spectra provide excellent agreement with experiment

Resumo/Abstract

Near-edge X-ray absorption fine structure (NEXAFS) spectroscopy is a powerful tool to probe the electronic structure of organic semiconductors, yet its interpretation remains challenging for chemically complex systems. In this work, we present a combined experimental and theoretical study of the carbon, nitrogen, and oxygen K-edge NEXAFS spectra of representative non-fullerene small molecule acceptors with A-D-A and A-π-D-π-A structure, such as ITIC and IDTBR, respectively. Angle-resolved NEXAFS measurements are complemented by TDDFT M06/6-311G(d,p) simulations, enabling a detailed assignment of spectral features in terms of core-level excitations, final-state symmetry, and spatial delocalization. The calculations reproduce the experimental spectra with good accuracy and reveal that the number of unoccupied states required for a reliable description strongly depends on the absorption edge, increasing systematically from carbon to nitrogen and oxygen. By correlating transitions across different edges, we show that identical final states can be probed from distinct core levels when heteroatoms are embedded within a conjugated backbone, providing complementary information on the unoccupied electronic structure. Angular-dependent measurements further allow the determination of preferential face-on orientation for these systems. The application of an artificial electric field over the calculated transitions allowed the variation in intensity of the experimental peaks to be reproduced with excellent accuracy, facilitating their understanding and attribution. By providing a unified interpretation of experimental NEXAFS spectra across multiple edges, this work offers new insights into the electronic structure of these acceptors and establishes a robust framework for analyzing core-level excitations in complex organic materials.



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In Situ Formation of Silver Nanoparticles in Mesoporous Silica Coatings for Antimicrobial Urinary Catheters

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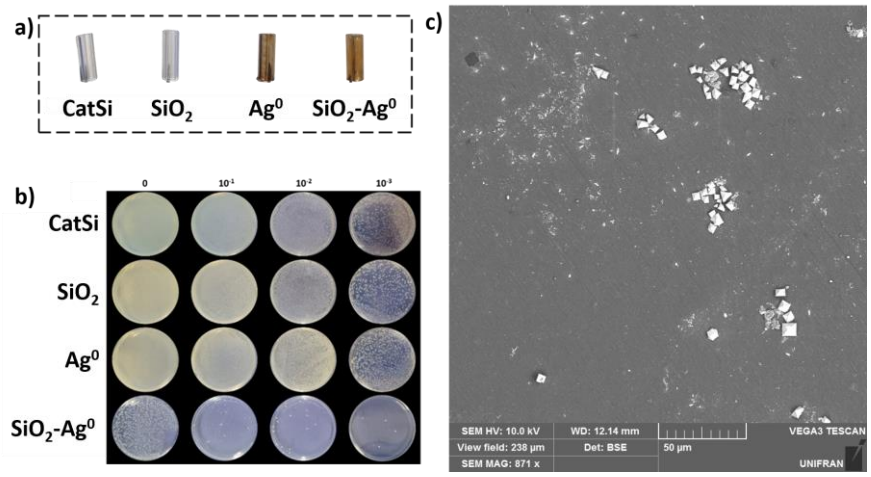
Palavras Chave:*Dip-coating,Silicone urinary catheters,Antimicrobial coatings,Catheter-associated urinary tract infections (CAUTIs),Biofilm inhibition*

Highlights

An antimicrobial coating of mesoporous silica with*in situ*formed silver nanoparticles was developed for urinary catheters, inhibiting biofilm and offering a strategy to reduce CAUTIs.

Resumo/Abstract

Catheter-associated urinary tract infections (CAUTIs) represent a serious public health problem and are frequently related to biofilm formation on the surface of these devices. In view of the increasing inefficacy of conventional antimicrobials, silver nanoparticles (AgNPs) have emerged as a promising strategy due to their broad spectrum of action and low risk of microbial resistance development. This project aimed to develop an antimicrobial coating for urinary catheters based on a mesoporous silica matrix incorporated with AgNPs. The mesoporous silica was synthesized by acid catalysis and deposited onto silicone catheters using the dip-coating technique. Subsequently, AgNPs were formed*in situ*within the matrix through the silver mirror reaction, using formic acid as the reducing agent. The removal of CTAB by solvent treatment was confirmed by FTIR, while UV–vis spectroscopy and scanning electron microscopy (SEM) analyses revealed the effective incorporation of prismatic-shaped silver nanoparticles into the silica matrix. In addition, antimicrobial assays were performed to evaluate the coating efficacy against*Escherichia coli*ATCC 25922. The developed coating inhibited biofilm formation, offering an innovative solution to reduce CAUTIs and improve patients' quality of life.



catheter segments coated with SiO_2 and/or Ag^0, biofilm test, and SEM-BSE image of prismatic Ag NPs

Agradecimentos/Acknowledgments

CAPES, CNPQ, FAPESP

INVESTIGAÇÃO DA BIOMASSA Clitoria fairchildiana R.A. HOWARD COMO REFORÇO PARA FERTILIZANTES COMERCIAIS: CARACTERIZAÇÃO E INTERAÇÃO FÍSICO-QUÍMICA.

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Palavras Chave:*Clitoria fairchildiana,fertilizantes,biomassa*

Highlights

Valorization of*Clitoria fairchildiana*biomass (leaves, seeds, and pods) as sustainable nutrient matrices.

Resumo/Abstract

Devido à baixa eficiência no uso de nutrientes em termos de solubilização e degradação associada à lixiviação, pesquisas demandam o desenvolvimento de tecnologias que possam melhor fixar esses fertilizantes no solo. Este trabalho tem a proposta de investigar se a presença de uma biomassa oriunda da espécie florestal Clitoria fairchildiana (F-folhas; S-sementes e V-vagens) pode ser aplicada como matriz de suporte para os fertilizantes comerciais. Usou-se como fertilizantes modelo os encontrados no mercado do tipo MAP e SSP. A coleta e armazenamento da biomassa segue o procedimento já estabelecido no grupo de pesquisa, três proporções foram propostas, mantendo fixa a massa dos fertilizantes e variando as proporções entre folha, vagem e semente (1:2, 1:3 e 1:4). O material gerado foi caracterizado por EDX, FTIR. A análise centesimal revelou um gradiente de estabilidade térmica, com teores de carbono fixo superiores nas V(10,68%), S(10,5%) e F(6,9%) indicando que a presença de lignina é mais acentuada nas vagens e sementes. O mapeamento por EDX, evidenciou que o MAP é rico em fósforo (77,4%) e pobre em cálcio (5,1%), enquanto o fertilizante modelo SSP é rico em cálcio (51,3%) e fósforo (13,9%). Dentre as proporções estabelecidas, foi possível observar que a F apresentou melhores resultados, favorecendo o enriquecimento de cálcio à medida que aumentava a proporção. O cálcio da F reage com o fósforo do fertilizante, maximizando a formação de complexos de fosfato de cálcio na superfície das fibras das folhas, favorecendo assim o enriquecimento dessa biomassa no fertilizante para o tipo MAP, já o potássio presente em V e S pode atuar como contra-íon para o fosfato, uma vez que S, por possuir um grupamento amida, favorece a liberação controlada dos íons, corroborando com os resultados obtidos no FTIR, confirmando a presença de grupos carboxilatos capazes de ancorar íons minerais. Conclui-se que a matriz F 1:4 sugere otimizar o MAP via oclusão, elevanto o teor de cálcio.

Agradecimentos/Acknowledgments

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Ligand-Controlled Chiral Recognition in Nanoparticle-Human Serum Albumin Interactions: Molecular Dynamics Simulation

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Palavras Chave:*Chiral Nanoparticles; Protein-Nanoparticle interactions, Human Serum AlbumiMolecular Dynamics Simulation,Chiral Nanoparticles, Protein-Nanoparticle interactions, Human Serum Albumin, Molecular Dynamics Simulation,Chiral Nanoparticles,Protein-Nanoparticle interactions,Human Serum Albumin,Molecular Dynamics Simulation*

Highlights

Chiral nanoparticles with carbohydrate or peptide ligands were studied; carbohydrate ligands showed enantioselective HSA binding (L-NP only); peptide ligands showed non-enantioselective binding.

Resumo/Abstract

Molecular dynamics (MD) simulations were employed to investigate the interaction between human serum albumin (HSA) and two classes of chiral inorganic nanoparticles differing in surface ligand chemistry: Mn_3O_4 nanoparticles functionalized with mannonic acid (carbohydrate-based ligand) and $Ni(OH)_2$ nanoparticles functionalized with glutathione (peptide-based ligand). For each system, nanoparticles in D, L, and racemic forms were simulated. Each simulation box contained four nanoparticles of identical chirality interacting with a single HSA molecule and was simulated for one microsecond using the CHARMM36 force field implemented in GROMACS 2025.1.

The two nanoparticle systems exhibited distinct enantioselective interaction behaviors with HSA. Carbohydrate-functionalized Mn_3O_4 nanoparticles displayed strong enantioselectivity, with the L-form showing persistent binding, while the D-form showed no stable interaction. These interactions were spatially localized and preferentially involved specific HSA domains. In contrast, peptide-functionalized $Ni(OH)_2$ nanoparticles showed no pronounced enantioselectivity, as both chiral forms interacted with HSA. In this case, interactions were distributed over multiple protein domains and differed primarily in interaction strength.

Overall, the results indicate that the chemical nature of the surface ligand critically modulates enantioselectivity, interaction localization, and domain preference in HSA–nanoparticle systems, highlighting ligand chemistry and chirality as key parameters in chiral nano–bio interactions.

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Lignin/Cellulose Microparticles as Intelligent Nutrient Release Devices

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Palavras Chave:*Agriculture, Biopolymers, Lignocellulosic Materials, Spray-drying.*

Highlights

The misuse of fertilizers causes environmental impacts. Sustainably produced EEFs reduce them. Lignocellulose/MAP particles were spray-dried. Microcapsules improve nutrient retention and release.

Resumo/Abstract

The Industrial Revolution (1760) marked a new era characterized by increased food demand due to population growth. Initially, the use of fertilizers proved efficient; however, improper application results in nutrient losses through leaching and volatilization, causing environmental impacts such as eutrophication. In the context of Sustainable Development Goals 2 and 12, this work aimed to develop lignocellulosic microparticles containing monoammonium phosphate (MAP) for use as enhanced efficiency fertilizers (EEFs) or as fillers in an additional matrix. EEFs reduce nutrient losses and environmental impacts by gradually releasing nutrient. Renewable and biodegradable biopolymeric matrices, such as microfibrillated cellulose (MFC) and lignin (Kraft lignin – LK and sodium lignosulfonate – LS), were combined with MAP. Microparticles were obtained by spray drying using double-fluid (2FN) and triple-fluid (3FN) nozzles, forming microspheres (Ms) and microcapsules (Mc), respectively. The microparticles were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and nutrient release kinetics in water. Particles produced with the 2FN nozzle showed a higher process yield (57.20%) but rapid nutrient release (~100% in 30 min). In contrast, microcapsules obtained with the 3FN nozzle and coated with LK exhibited spherical morphology and gradual nutrient release (~100% in 150 min). The analyses confirmed MAP incorporation and greater thermal stability in LK-containing formulations. Due to its hydrophobic character, LK coatings showed greater ionic retention, whereas LS coatings favored faster nutrient release. The LK:MFC.MAP_Mc formulation stood out for its prolonged release, reaching 100% at 180 min. Thus, lignocellulosic microparticles produced by spray drying represent a promising strategy for sustainable EEFs development with reduced environmental impact.

Agradecimentos/Acknowledgments

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Lignin extracted from coffee husk as a functionalizing and stabilizing agent for copper nanoparticles

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Palavras Chave:*Lignin nanoparticle,,Coffee processing residues,,Agro-industrial waste valorization,,Solvent/Antisolvent technique,Nanotechnology application*

Highlights

Lignin functionalization modifies the properties of CuNP and reduces aggregation, improving nanoparticle dispersion and colloidal stability.

Resumo/Abstract

The residues obtained from coffee processing are rich in nutrients, becoming a promising source of lignocellulosic material for the production and extraction of relevant compounds. One relevant compound is lignin that is rich in phenolic compounds with great applications. Concomitantly, copper nanoparticles present diverse applications, with emphasis on the agriculture as a pest controlling agent and fertilized. The functionalization of lignin with copper nanoparticles is a promising strategy in the control of agricultural phytopathogens as well as for the fertilization of plants. The lignin nanoparticle provides colloidal stability and dispersion for the copper nanoparticles, promoting the slow release of the nutrient. In this study, the effect of lignin as a functionalizing and stabilizing agent for copper nanoparticles (CuNP) was investigated using classical characterization techniques such as UV-Vis, DLS, TG, SEM imaging. The nanoparticles were synthesized and functionalized with the lignin nanoparticles in which lignin acts as a reducing and stabilizing agent due to its structure rich in phenolic compounds. The analysis revealed that the lignin acts as a coating over the CuNP, while also improving the dispersion of the nanoparticles and decreasing aggregation. Lignin plays a fundamental role in controlling nanoparticle aggregation and enhancing colloidal stability. In conclusion, lignin extracted from coffee husk represents a sustainable and efficient functionalizing agent for CuNP, contributing to the valorization of agroindustrial waste within a bioeconomy framework.

Agradecimentos/Acknowledgments

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Low Reynold's number fluid flow controlled by metachronal wave in magneto-driven cilia surfaces for mucociliary clearance

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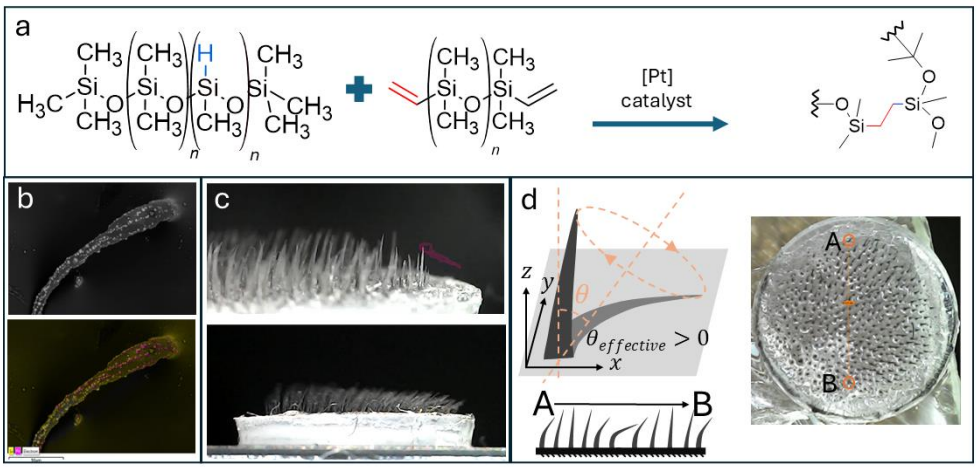
Palavras Chave:*Magnetic cilia,Silicone surface,Tracheal stents,Mucociliary clearance*

Highlights

Magnetic fields was used to create metachronal waves and propel low Re fluids.
A template-free self-assembly method was used to engineer silicone-based ciliated surfaces.

Resumo/Abstract

Ciliated cells on the surface of trachea and the periciliary layer consisting of mucin glycopolymers, and the protective mucus layer forms the mucociliary clearance system, the major innate defense system of the airway. The cilia should beat in a metachronal manner to move unidirectionally the mucus. Here, we aim to engineer bioinspired magnetically responsive cilia surfaces functionalized with glycopolymers that mimics the composition of the natural mucin. The method consists in a template-free magneto-driven self-assembly approach where a suspension of carbonyl iron particles (~1.6 µm) and polydimethylsiloxane elastomer precursors (PDMS, biomedical grade) in ethyl acetate is prepared creating a magnetic fluid and cured (90 °C) on the permanent magnets (~0.22 T) surface to form a ciliated field-oriented surface. The PDMS surfaces were submitted to atmospheric pressure argon plasma promoting the formation of oxygenated groups (-OH) for further reactions until the polymerization of micuin-mimetic glycopolymers on the surface. High resolution images and videos were used to obtain the phase difference (0.2718 x 2π radians) and metachronal wavelength (19.536 mm) of the cilia array and the capacity of propel in two directions a mucus-mimetic fluid with low Reynold's number. The results suggest success in the obtention of high cilia (~900 µm), chemical functionalization of silicone-based surfaces, and the creation of 3D beating patterns by permanent magnets approach, able to control the velocity and direction of fluid flow in mucus-mimetic solution. The control of all these parameters could be applied to create smart tracheal stents with self-cleaning capacity promoting mucociliary clearance.



(a) Hydrosilylation reaction. (b) SEM and EDS images. (c) Cilia trajectory. (d) Metachronal wave.

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP, Brazil; process n°. 2022/14809-5). Author Sousa acknowledges FAPESP (grant n° 2024/15295-0).

LUMINESCENT THIN FILMS FOR APPLICATIONS IN LIGHT-EMITTING SYSTEMS

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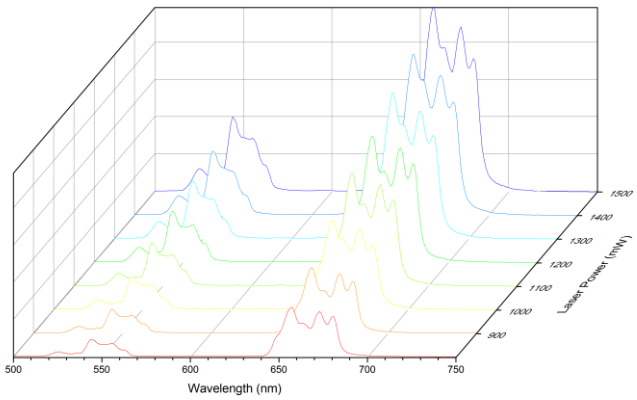
Palavras Chave:*GAG,GAP,bioimaging,photovoltaic cells,luminescence*

Highlights

Lanthanide-ion-doped aluminum matrix coated with silica shell for radiation-emitting systems

Resumo/Abstract

Technological advances have brought about the need for the development of increasingly sophisticated radiation-emitting systems, which may operate both in energy generation and in devices for biological labeling. In this context, research on materials with intrinsic luminescent properties has been widely explored, as they exhibit the ability to absorb and emit radiation at different wavelengths. This work aims to investigate the preparation of mixed aluminum–gadolinium oxides doped with lanthanide ions Ln^{3+} (Ln^{3+} = Eu^{3+}, Er^{3+}, Yb^{3+}, Nd^{3+}). The matrix was synthesized using the non-hydrolytic sol–gel methodology and subsequently coated with silica, forming a core–shell system. The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and photoluminescence (PL). For application in thin films, the material was suspended in ethanol and deposited in glass substrate using the dip-coating technique. X-ray analyses showed the disappearance of the characteristic diffraction peaks of the mixed oxide matrix, accompanied by the growth of an amorphous halo characteristic of silica, indicating its formation as a shell over the matrix. This behavior is corroborated by SEM images, in which a clear difference in particle texture with and without the silica shell can be observed. Photoluminescence results indicate that, when applied onto a substrate, the matrix exhibits changes in its luminescent behavior, suggesting modifications in the local environment of the ions. The photoluminescent images obtained from the aluminum–gadolinium matrix doped with Ln^{3+} (Eu^{3+}, Er^{3+}, Yb^{3+}) ions can be observed in Figure 1.



Upconversion emission spectrum excited at 980 nm of the aluminum–gadolinium Ln-doped sample

Agradecimentos/Acknowledgments

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Mechanochemical synthesis of ordered mesoporous carbons from biomass for the adsorption of large emerging contaminants

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Palavras Chave:*Mechanochemistry,Tannin,Solvent-free,sustainability,ivermectin adsorption*

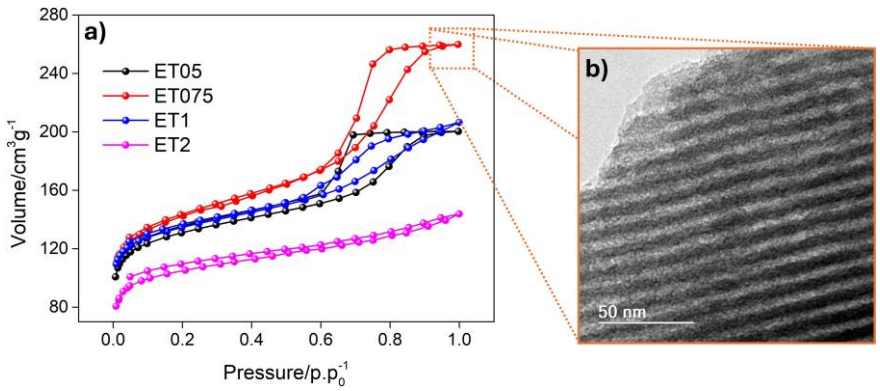
Highlights

Solvent-free mechanochemical synthesis of tannin-derived carbons.
Tuning mesoporosity via F127 ratio control.
Efficient adsorption of large emerging contaminants like ivermectin.

Resumo/Abstract

This work investigates the effect of F127 surfactant content on the synthesis of mesoporous carbons derived from tannin extract, aiming at the adsorption of the large emerging contaminant ivermectin. The materials were prepared using a solvent-free mechanochemical method, varying the tannin:F127 ratio to 1:0.5, 1:0.75, 1:1, and 1:2, and were named ET05, ET075, ET1, and ET2, respectively. N_2 physisorption isotherms revealed that reducing the surfactant amount promotes the formation of materials with higher mesopore volume, changing the isotherm type from I to IV. This trend was accompanied by an increase in average pore diameter from 3.1 to 9.5 nm. The material synthesized at the 1:0.75 ratio exhibited the highest surface area (525 $m^2\ g^{-1}$) and total pore volume (0.402 $cm^3\ g^{-1}$), with a predominance of mesopores. Transmission electron microscopy (TEM) images confirmed the presence of ordered and well-distributed pores, especially for ET075. A preliminary adsorption study showed that all materials completely removed ivermectin from the system. To better understand the adsorption mechanisms, two materials with distinct porosities (ET075 and ET2) were selected for kinetic and isotherm studies. Both exhibited similar adsorption capacities at low concentrations; however, at higher concentrations, the mesoporous material (ET075) achieved a higher maximum adsorption capacity (≈99%). Moreover, the adsorption kinetics were faster for the material with larger pore sizes and volumes. These findings demonstrate that the adsorption performance of large emerging contaminants depends not only on surface area but also on the presence and accessibility of mesopores, highlighting the importance of pore-structure control in biomass-derived carbon materials.

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a) N2 physisorption isotherm for materials; b) Transmission electron micrograph for ET075.

Agradecimentos/Acknowledgments

CNPq, CAPES, Fapemig, MOVER, CTNANO/UFMG, Centro de Microscopia da UFMG, JOVEMPESQ/UFBA, RSC, INCT MIDAS, Grutam/UFMG.

Metal Coordination in Starch-Based Natural Polymer Films: Ion–Polymer Interactions and Physicochemical Properties

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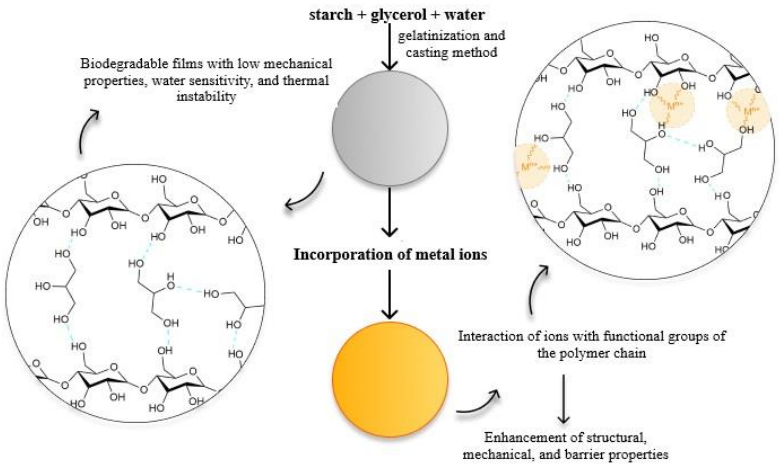
Palavras Chave:*Biopolymers; Ionic crosslinking; Metal coordination; Physicochemical properties*

Highlights

Investigation of metal coordination as a strategy for structural modification in starch-based films. Analysis of metal–starch interactions and their physicochemical effects.

Resumo/Abstract

Plastic pollution caused by conventional petroleum-based plastics has driven the search for biodegradable materials derived from renewable sources. In this context, starch emerges as an abundant and low-cost biopolymer; however, starch films exhibit limitations related to mechanical resistance, thermal stability, and sensitivity to water. Metal coordination is a promising strategy to overcome these drawbacks by promoting additional physicochemical interactions between polymer chains without covalent backbone modification. This work investigates the incorporation of metal ions into glycerol-plasticized starch films, focusing on interactions between metal centers and polymer functional groups. Films are prepared by starch gelatinization of starch followed by casting method, and characterized for mechanical, thermal, and structural properties using infrared spectroscopy, X-ray diffraction, tensile testing, thermogravimetric analysis, solubility and swelling tests. The FTIR spectra of films containing a transition metal showed profiles similar to the control (without metals), indicating preservation of the starch chemical structure. Subtle variations in the O–H band suggest local coordination interactions without detectable formation of new covalent bonds. RGB colorimetric analysis revealed systematic color changes upon transition metal incorporation. A calibration curve was obtained by varying the concentration of the metals in the films. This approach enables evaluation of metal coordination as a physical crosslinking mechanism influencing polymer matrix organization and physicochemical properties. The study contributes to the understanding of metal–biopolymer interactions in starch-based systems, with potential application in the development of biodegradable materials.



Representation of metal coordination in starch films and its structural influence.

Agradecimentos/Acknowledgments

The authors are grateful for the financial support by the Brazilian agencies FAPESP (2025/21280-9 and 2025/09383-7), Capes and CNPq.

Metastable molybdenum phases as sensors for MVOCs detection

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Palavras Chave:*Gas sensors, Metastable phases, Molybdenum oxide, Triethylamine, MVOCs.*

Highlights

High selectivity toward Triethylamine (TEA) detection.
High response for TEA detection at 100 ppm, even at low concentrations.
Low operating temperatures (150 °C) with reduced power consumption.

Resumo/Abstract

This research aims to study molybdenum-based structures for the fabrication of conductimetric sensors intended for the detection of microbial volatile organic compounds (MVOCs). The precursor for metastable MoO_3 structures was synthesized by microwave-assisted hydrothermal method, via precipitation of H_2MoO_3 in an acidic medium, yielding hydrated $MoO_3 \cdot 1/2H_2O$, a mixture of monoclinic and hexagonal phases. The thermal decomposition of the precursor allowed the obtaining of the hexagonal (H-MoO_3) and orthorhombic (O-MoO_3) phases, characterized by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR), confirming the formation of the respective phases, with indexing of the crystalline planes and identification of the vibrational stretching characteristic of the Mo-O bond. The pure phases were morphologically characterized by scanning electron microscopy (SEM), revealing distinct morphologies: rod-shaped macrostructures for the hexagonal phase and plates for the orthorhombic phase. The hydrated phase presented a mixed morphology, combining both structures. The sensors were evaluated for the detection of different MVOCs (acetone, 2-butanone, ethanol, ethyl acetate, 1-pentanol, benzene, toluene, xylene, and triethylamine) at operating temperatures between 150 and 400 °C. The sensor based on the orthorhombic phase (O-MoO_3) showed the best performance and high selectivity for triethylamine (TEA) detection at 350 °C, with a maximum response of 672.64. At low temperatures (≤150 °C), selectivity for TEA is enhanced, making it the only VOC detected in this range.

Agradecimentos/Acknowledgments

I would like to thank CAPES for the doctoral scholarship granted (Process No. 88887.008706/2024-00), FAPESP (Process No. 2020/06421-1; 2022/05381-1; 2024/03388-4), CNPq (Process No. 305542/2024-9).

Methacrylated Cellulose Nanocrystals as a Bio-Based Reinforcing Additive for 3D-Printable Dental Resins

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Palavras Chave:*: Methacrylated cellulose nanocrystals, additive manufacturing, 3D printing, dental materials, polymer composites,Methacrylated cellulose nanocrystals, additive manufacturing, 3D printing, dental materials, polymer composites*

Highlights

CNCs are promising sustainable, multifunctional dental materials.
Solvent exchange is an effective method for CNC surface modification.
mCNC additive improved the homogeneity of the commercial resin.

Resumo/Abstract

Cellulose nanocrystals (CNCs) are promising sustainable, multifunctional components for dental materials due to their versatility and natural abundance. On the other hand, acrylate-based materials such as poly(methyl methacrylate) are widely used in dentistry owing to their established performance and ease of processing. This work bridges these two material classes by exploring the use of methacrylated cellulose nanocrystals (mCNCs) to enhance and diversify the properties of conventional resins. The mCNCs were synthesized from commercial CNCs via a solvent exchange process, sequentially using water, ethanol, acetone, and poly(ethylene glycol) methyl ether methacrylate, followed by 30 minutes of sonication for dispersion. These mCNCs were incorporated as reinforcing fillers into two commercial acrylate-based 3D-printable resins at concentrations of 0.5, 0.75, and 1.0 wt%. A comprehensive investigation of the rheological properties, mechanical performance, and viscoelastic behavior of the cross-linked formulations was conducted. The results confirmed that solvent exchange is an effective method for CNC surface modification. The addition of 0.75 wt% mCNCs increased the tensile strength to 100 MPa ± 4.6. Furthermore, the biobased additive improved the homogeneity of the commercial resin, as evidenced by reduced variability between samples with and without the additive. All formulations absorbed light at 405 nm with transmittance values up to 70%. SEM images revealed a strong interface between the filler and the resin matrix. These findings indicate that mCNCs are a promising bio-based reinforcement for 3D-printable dental formulations using vat polymerization techniques such as stereolithography (SLA) or digital light processing (DLP).

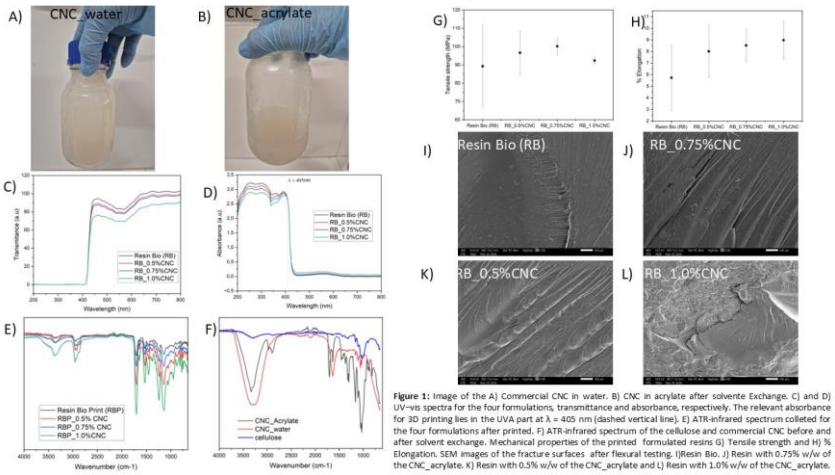


Figure 1: Image of the A) Commercial CNC in water. B) CNC in acrylate after solvente Exchange. C) and D) UV-vis spectra for the four formulations, transmittance and absorbance, respectively. The relevant absorbance for 3D printing lies in the UVA part at λ = 405 nm (dashed vertical line). E) ATR-infrared spectrum colleted for the four formulations after printed. F) ATR-infrared spectrum of the cellulose and commercial CNC before and after solvent exchange. Mechanical properties of the printed formulated resins G) Tensile strength and H) % Elongation. SEM images of the fracture surfaces after flexural testing. I)Resin Bio. J) Resin with 0.75% w/w of the CNC_acrylate. K) Resin with 0.5% w/w of the CNC_acrylate and L) Resin with 1.0% w/w of the CNC_acrylate.

A and B) Picture. C and D) UV-Vis. E and F) ATR-FTIR. G and H) Mechanical test. I, J, K and L) SEM

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FAPES, UFES, UNICAMP, LABMAT, LMC, NCQP/UFES.

Modulation of optical emission in Yb/Tm/Eu core@shell nanoparticles driven by surface acoustic waves

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Palavras Chave:*lanthanide-doped nanoparticles,surface acoustic waves,energy transfer upconversion*

Highlights

Surface acoustic waves strongly enhance Tm and Eu emission intensities at low temperature, with intensity gains reaching two orders of magnitude.

Resumo/Abstract

Lanthanide (Ln) ions are known for their optical properties that are highly sensitive to external stimuli. Surface acoustic waves (SAWs), in turn, generate strain and piezoelectric fields that can modulate optical emission in different nanostructures. Recently, we employed the Er optical emission in Yb/Er-doped core@multishell nanoparticles (NPs) to locally probe the SAW-induced heating at high acoustic powers via luminescent nanothermometry [1]. Here, we investigate the optical response of Yb/Tm/Eu-doped core@shell NPs integrated in a SAW delay line. Using upconversion spectroscopy, we analyzed the recombination dynamics of the ions under the influence of SAWs propagating on $LiNbO_3$ substrates. The Yb^{3+} ions were optically excited, enabling energy transfer (ET) to Tm^{3+} and Eu^{3+}, and the corresponding emissions were monitored. At 5 K, we observed a strong enhancement of the Tm^{3+} and Eu^{3+} emission intensities (up to two orders of magnitude), accompanied by a modification of the excitation power law. Additionally, by exciting the Tm^{3+}, we observed a quenching of the Yb^{3+} emission upon SAW application, indicating that the SAW directly influences the ET channels between the Ln ions. Time-resolved measurements indicated that the mechanical deformation of the SAW does not affect the local symmetry, as evidenced by the Eu^{3+} emission upon SAW, showing that the deformation does not modify the optical selection rules. The results point to a possible enhancement in the ET efficiency between Yb^{3+} and Tm^{3+} mediated by coherent SAW phonons, although the microscopic mechanism describing this coupling is still under investigation. Nonetheless, the considerable enhancement of the emission intensity experimentally detected in the Tm-doped NPs creates very interesting prospects for a dynamic and on-demand control of the optical emission of Ln-based NPs using acoustic fields.

[1] P. B. Pinto et al.*Advanced Optical Materials*,**13**, 2403497 (2025)

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Numbers 2025/17225-2, 2021/06803-4, 2022/03323-4, 2023/00191-2, 2021/0811-2.

Molten salt synthetic method for alkaline earth metal aluminates

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Palavras Chave:*Molten salt,persistent luminescence,aluminates,phosphors*

Highlights

A new molten salt method for (Ca,Sr,Ba)Al_2O_4 obtaining pure and doped luminescent material

Resumo/Abstract

Alkaline earth metal aluminates have been extensively studied as phosphor matrices since their description, with particular interest in high luminescence and long persistence.[1] Since then, a better understanding of the basic persistent luminescence mechanism has been reached.[2] However, little is known about how the synthetic method could influence luminescence, as new methods may yield novel morphologies as well as improved luminescent properties. In this work, $CaAl_2O_4$, $SrAl_2O_4$ and $BaAl_2O_4$ were obtained using a molten salt method with a KCl/NaCl flux in different salt/oxide ratios.The formed phases (figure 1.a) and their morphologies (figure 1.b) were identified by XRD, SEM and TEM, respectively. The use of different solvents for salt removal was also investigated, revealing its influence on the final product morphology. Inclusion of different dopants (Eu^{3+}, Tb^{3+} and Pr^{3+}) was achieved after a two-step calcination process, with a similar intermediate forming for all aluminates after the first heat treatment.The obtained materials show single-phased compounds with good purity for Ca and Ba aluminates, and a mixture of hexagonal and monoclinic $SrAl_2O_4$. Their luminescence is being studied by spectrofluorimetry, exhibiting the typical rare-earth luminescence.

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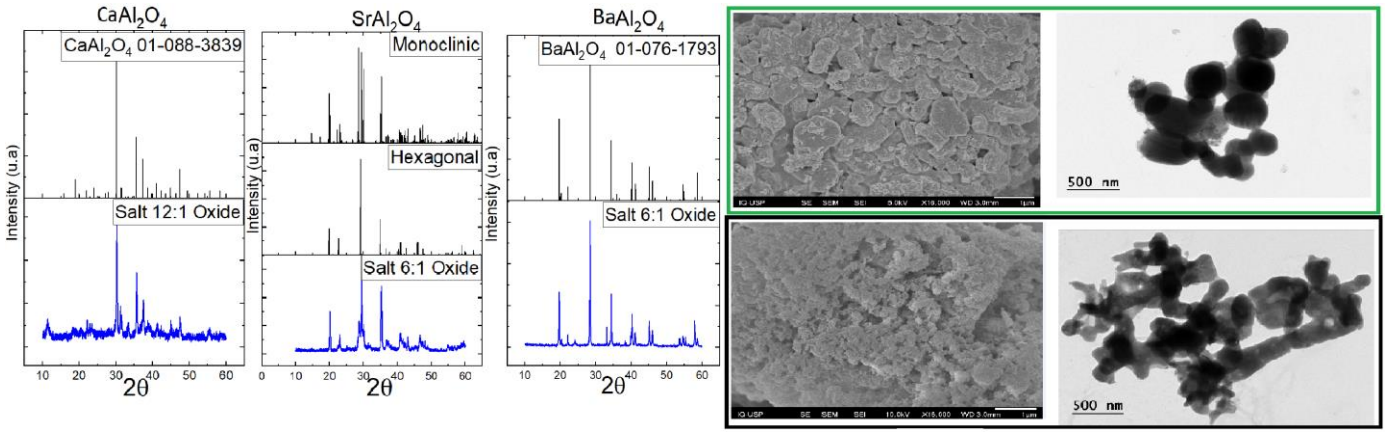


Figure1.a) XRD pattern; Figure 1.b) SEM and TEM of (green) glycerin and (black) water cleaned

Agradecimentos/Acknowledgments

We acknowledge the Brazilian agencies CAPES, CNPq and FAPESP for the financial support. The images were made using IQ-USP Central Analítica facilities and assistance.

Molybdenum Disulfide 2D: A Side-by-Side study of Commercial and Synthed Forms

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Palavras Chave:*Molybdenum disulfide, thin film, nanomaterials, liquid-liquid interface route, 2D materials,Molybdenum disulfide,, thin film,thin film,nanomaterials,liquid-liquid interface route,2D materials*

Highlights

Synthesized MoS_2 shows higher exfoliation yield and stability. The LLIR method to fabricate transparent and homogeneous thin films. Production of laboratory-synthesized MoS_2 costs less.

Resumo/Abstract

Molybdenum disulfide (MoS_2) is a 2D material with unique electronic and optical properties, whose performance depends on the efficiency of its exfoliation and processing. This work presents a systematic comparative study between MoS_2 synthesized in our laboratory (MoS_2-S) and a commercial counterpart (MoS_2-C). MoS_2-S was obtained via thermal treatment of amorphous precursors, resulting in smaller flakes (~70 nm) with higher density of structural defects and active edges, as shown by SEM and Raman analyses. In contrast, MoS_2-C presented larger flakes (~600 nm) and high crystallinity. Both materials were exfoliated in liquid phase by ultrasound in different solvents. The results demonstrated that MoS_2-S disperses more easily, with concentrations up to 4.5 times higher than MoS_2-C, and stability was observed for 30 days. Analytical curves were established through UV-Vis measurements to quantify the exfoliation yield. Using the liquid-liquid interface route (LLIR), developed in our group, we fabricated transparent and homogeneous thin films on solid substrates. The MoS_2-S films exhibited superior optical quality, with thickness and absorbance linearly controllable with the concentration of the initial dispersion. In contrast, MoS_2-C resulted in heterogeneous films that were difficult to process. The production cost of MoS_2-S proved to be lower than that of the commercially available sample, positioning it as a highly competitive alternative for applications in energy storage devices and sensors.

Agradecimentos/Acknowledgments

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Multication hybrid lead bromide perovskites: octahedral framework distortions and their impact on optoelectronic properties

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Palavras Chave:*hybrid perovskites, lead bromide, multications, solution-processed method, organic-inorganic chemistry*

Highlights

The versatility of hybrid perovskites paired with compositional engineering enables fine tuning of optoelectronic properties via stoichiometric control and organic-cation-driven ocahedral distortions.

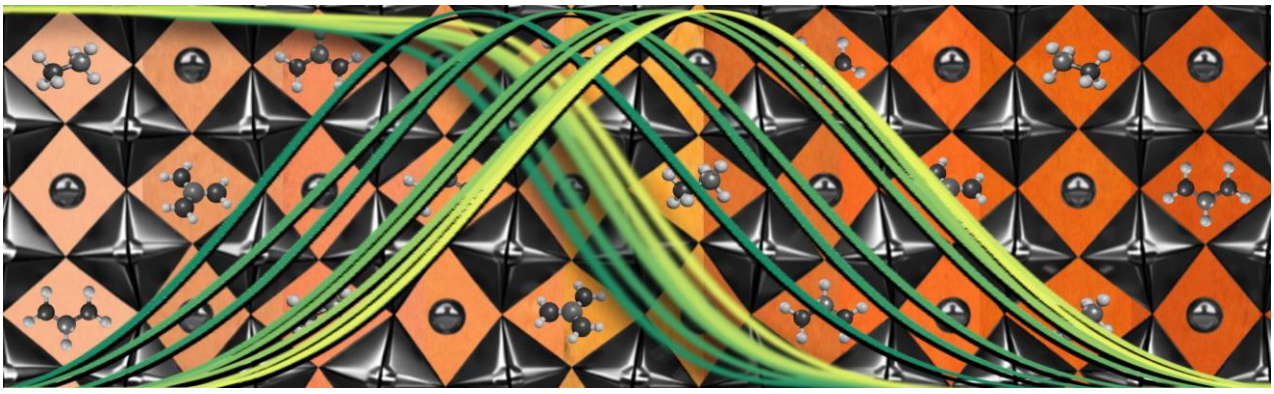
Resumo/Abstract

The development of advanced semiconductor materials is strategic for Brazil's scientific and technological sovereignty, particularly in energy, optoelectronics, and photonics. This work reports the synthesis and characterization of hybrid lead bromide perovskites with different A-site cations, including methylammonium (MA^+), formamidinium (FA^+), guanidinium (GA^+), cesium (Cs^+), and selected multication compositions, aiming to elucidate the influence of A-site chemistry on crystal structure and optoelectronic properties.

The materials were synthesized via a simple and low-cost solution-based route under acidic conditions, without coordinating ligands or stabilizing agents. This approach reduces process complexity and production costs, while minimizing solvent use and enhancing scalability for functional materials development.

Systematic modulation of the A-site cation led to distortions in the $[PbBr_6]^{4-}$ octahedral framework, as evidenced by X-ray diffraction (XRD), resulting in symmetry changes and microstructural variations. Morphological analysis indicated a composition-dependent microstructural organization. Optical properties were investigated using UV-Vis absorption spectroscopy and time-resolved photoluminescence (TRPL), revealing variations in bandgap energy, radiative efficiency, and charge-carrier recombination dynamics. FTIR measurements confirmed specific interactions between organic cations and the inorganic framework.

These results demonstrate that chemical engineering of the A-site is an effective strategy to fine-tune optoelectronic properties and enhance the stability of hybrid perovskites without altering the halide or metal composition. This study contributes to the fundamental understanding of halide perovskites and highlights the role of accessible chemical routes for strengthening functional materials research with potential applications in energy-related devices.



A-site cation effect on octahedral distortions and optoelectronic properties of hybrid perovskites.

Agradecimentos/Acknowledgments

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Nanocomposite-based soil conditioner: Starch/Nanoclay

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Palavras Chave:*Soil conditioner,Nanoclay (NC),Thermoplastic starch (TPS),Nanocomposites,Agriculture*

Highlights

The addition of NC in the TPS matrix improved physical-chemical properties;

The TPS/NC7% sample showed a better NPK ion leaching, biodegradability and seedling growth.

Resumo/Abstract

Projections indicate continuous population growth, leading to a greater demand for food, pressuring increasingly exhausted arable land. Soil conditioners are proving to be a good alternative in the search for greater soil efficiency, increasing its productivity. Thermoplastic starch (TPS) presents interesting characteristics for this purpose, while nanoclay (NC) demonstrates potential to reinforce its polymeric network, generating new properties. These low-cost materials were combined for the development of optimized formulations in proportions of 3%, 5% and 7% (w/w) of NC in relation to TPS. FTIR results show that structural modifications occurred in the material when the two components were mixed, with greater intensity in TPS/NC7%, being visible in SEM images. The TPS/NC7% sample swelled the most compared to TPS and the others, especially in slightly acidic and neutral media, with 32%, 39%, and 21% swelling at pH 5, 7, and 9, respectively. It also had the lowest solubility, especially in slightly acidic and slightly basic media, being 30%, 25.4%, and 24.4% for pH 5, 7, and 9, respectively. The neutral pH of the nanocomposites can guarantee their use in a wide variety of soils. The cation exchange capacity (CEC) was also superior in the nanocomposites compared to TPS, with a higher value in TPS/NC7%, indicating greater availability of nutrients to the medium in which they were found. Performance tests of leaching, biodegradability, microbial activity, and planting show that TPS/NC7% is the composite that presents a better release of NPK ions, as well as a lower release of CO 2 and proliferation of microorganisms, and greater productivity in seedling growth, reducing the effect of dormancy in seeds. Thus, the TPS/NC7% composite stood out for improving not only the physical and chemical properties of the soil, but also for demonstrating economic viability and sustainability, contributing to more efficient and environmentally responsible agricultural practices.

Agradecimentos/Acknowledgments

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Nanocomposite thin films between PEDOT and gold nanoparticles - preparation and application study

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Palavras Chave:*Conductive Polymer, Nanoparticles, Thin Film, Nanocomposites*

Highlights

Preparation of nanocomposites between PEDOT and gold nanoparticles (AuNPs) through spontaneous reaction). Thin films obtained with different proportions and reaction times, in a single step.

Resumo/Abstract

In recent decades, materials science efforts aimed at developing new materials have grown significantly, as has the demand for systems with advanced functional properties. In this context, nanomaterials stand out, whose physical, chemical, and optical properties strongly depend on their size and morphology. Gold nanoparticles (AuNPs) are of great interest due to the presence of intense absorption bands in the visible spectrum, associated with surface plasmon resonance.Another group of materials widely studied are conductive polymers, poly(3,4-ethylenedioxythiophene) (PEDOT) stands out for its high electrical conductivity and good charge mobility, attributed to non-covalent interactions between its polymer chains. The combination of PEDOT and AuNPs makes it possible to obtain nanocomposites with synergistic properties, which can be synthesized in a single step, without the need for a solid phase.In this work, nanocomposites were prepared using the liquid-liquid interfacial route, which allows the formation of thin nanocomposite films at the interface between two immiscible solvents[1]. The two-phase systems consisted of an aqueous phase and an organic phase, containing $HAuCl_4$ and EDOT, respectively. Samples with different reaction times and molar ratios between the precursors were obtained.All samples were characterized by UV-Vis and Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS), and voltammetry. The results indicate the spontaneous polymerization of EDOT concomitant with the formation of AuNPs. Varying the EDOT/$AuCl_4^-$ molar ratio allowed controlling the size of the AuNPs and the electronic properties of the nanocomposites. Finally, the materials were evaluated in a photovoltaic cell system, exhibiting different resistance and electrical current values, which highlights their potential for applications in this type of device.

[1] Zarbin, A. J. G. Mater. Horiz. 2021, v. 8, p. 1409.

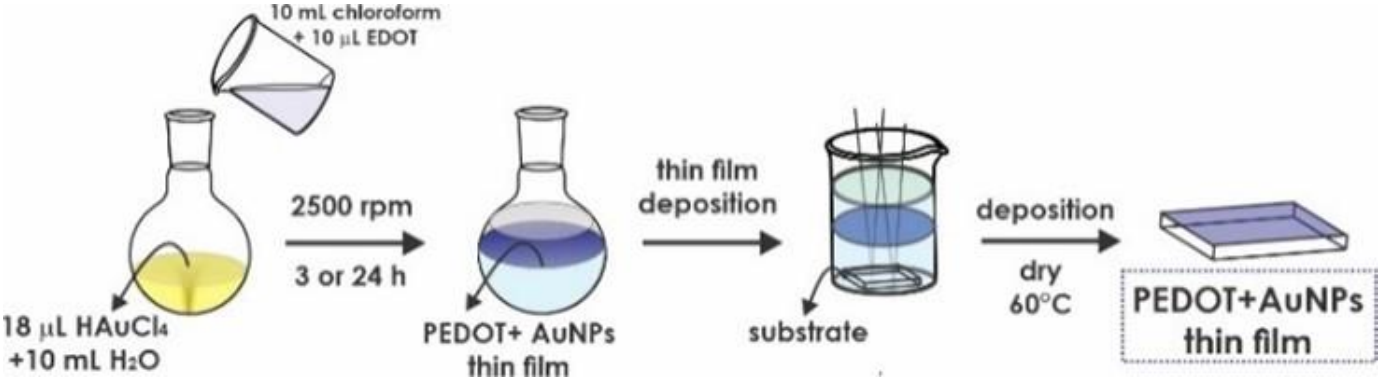


Figure: liquid-liquid interfacial methodology

Agradecimentos/Acknowledgments

CNPq, CAPES, INCT NanoVida, INCT Nanocarbono and UFPR Scientific and Technological Initiation Coordination.

Nanoesferas de carbono dopadas com nitrogênio um material eletroquímico sustentável para detecção de antibióticos em carne bovina

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Palavras Chave:*Sensor eletroquímico,eletroanálise,antibiótico,carne bovino,nanoesfera de carbono dopadas com nitrogênio*

Highlights

Nanoesferas de carbono dopadas com nitrogênio, sensor eletroquímico para antibiótico, sensor miniaturizado, nanomateriais sustentáveis

Resumo/Abstract

A presença de resíduos de antibióticos em carnes representa um risco significativo à saúde pública, o que torna indispensável um controle de qualidade rigoroso. No entanto, os métodos analíticos atualmente empregados são, em geral, dispendiosos, demorados e exigem infraestrutura laboratorial complexa. Neste contexto, o presente trabalho propõe o desenvolvimento de um método eletroanalítico rápido, sensível e de baixo custo para a detecção de antibióticos em amostras de carne, utilizando eletrodos impressos de carbono modificados com nanoesferas de carbono dopadas com nitrogênio (N-CSS) sintetizadas por um método hidrotérmico, empregando glicose, água e glutationa como precursores. O procedimento desenvolvido é simples, atóxico, de baixo custo e ambientalmente amigável. As sínteses foram realizadas a 160 °C, 170 ºC e 180ºC por diferentes tempos de reação (3, 4, 5, 6 e 7 horas), utilizando uma proporção massa:massa de 1:200 (glicose:glutationa). As amostras foram caracterizadas por microscopia eletrônica de varredura com canhão de emissão de campo (FEG-SEM) revelando partículas com morfologia esférica e diâmetros médios variando entre 311 ± 31 nm e 1169,6 ±355,36nm. O aumento do tempo e da temperatura de reação favoreceram o crescimento das nanoesferas resultando em um aumento progressivo do diâmetro médio das partículas. Esse comportamento pode ser atribuído ao aumento da energia cinética das moléculas no sistema, que promove maior frequência de choques efetivos. Com a modificação dos eletrodos de carbono com N-CSS, espera-se obter elevada performance analítica, com limites de detecção e quantificação adequados para a determinação de antibióticos em amostras de carne bovina, contribuindo para o desenvolvimento de uma alternativa sustentável, portátil e descentralizada para o controle de qualidade de alimentos.

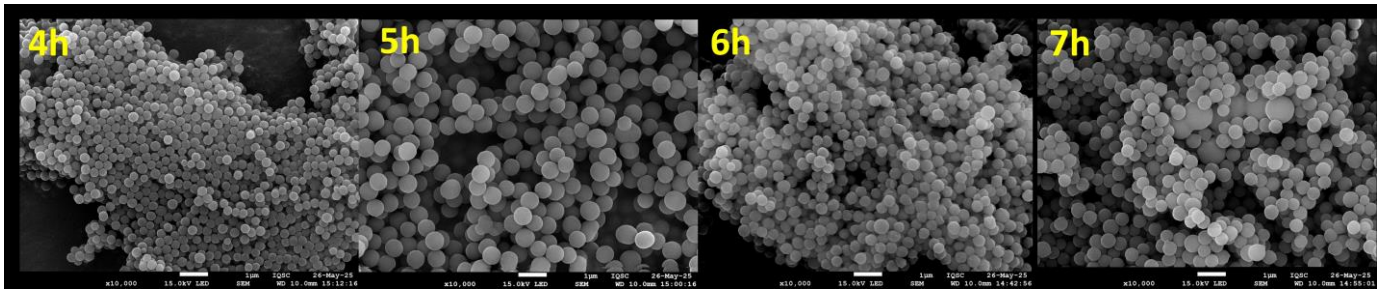


Imagem de Microscopia Eletrônica de Varredura das nanoesferas de carbono dopadas com nitrogênio

Agradecimentos/Acknowledgments

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Nanometric nickel-promoted Silicalite-1 for improved accessibility of bulky oxygenates

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Palavras Chave:*Silicalite-1,nanometric zeolite,nickel dispersion,microcapillarity,catalyst synthesis*

Highlights

Synthesis of nanometric Silicalite-1 to maximize Ni dispersion and minimize steric hindrance in HDO of bulky phenolics, investigating the interplay between diffusion path length and MFI channels.

Resumo/Abstract

Metal dispersion in microporous materials is enhanced during catalyst preparation due to capillarity effects associated with their textural properties. However, despite the high dispersion of active sites, the application of such materials in the conversion of biomass-derived compounds may be hindered by steric constraints and diffusion limitations, as pore dimensions are frequently smaller than the kinetic diameters of the reactants. While the MFI topology offers unique confinement effects, micrometric crystals can restrict the access of bulky oxygenates to internal active sites. Unlike aluminosilicates, pure Silicalite-1 provides a hydrophobic environment, ideal for the hydrodeoxygenation (HDO) of phenolic compounds. Therefore, this work investigated the synthesis of nanometric Silicalite-1 crystals (<100 nm) promoted with nickel (Ni), comparing them to their micrometric counterparts (≈1000 nm), to evaluate the impact of diffusion path length on metal dispersion and reactant accessibility to the active phase. Material characterization enabled the correlation of the accessible surface area with the kinetic diameters of the target molecules. Preliminary results indicate superior Ni dispersion within the nanometric matrix, suggesting enhanced accessibility for bulky molecules.

Agradecimentos/Acknowledgments

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Nanosized MFI Zeolite with Enhanced Water Tolerance

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Palavras Chave:*MFI,Synthesis,Zeolite,Nanoparticles*

Highlights

- MFI zeolites were obtained with crystal sizes ranging from 70 to 1200 nm.
- Nanosized MFI zeolite was synthesized with enhanced water tolerance promoted by tungsten incorporation.

Resumo/Abstract

Pure-silica zeolites possessing the MFI framework with crystal sizes ranging from 70 to 1200 nm were hydrothermally prepared by tuning synthesis parameters, including TPAOH saturation, crystallization time, and temperature. A systematic investigation was carried out to correlate crystal size with the structural and textural properties of silicalite-1.
To overcome the intrinsic hydrothermal instability commonly associated with nanosized MFI zeolites, tungsten was incorporated into the precursor solution to promote silanol healing and framework stabilization. The resulting nanosized sample exhibited enhanced water tolerance compared to the untreated MFI-70. Hydrothermal stability tests demonstrated that the tungsten-stabilized nanosized MFI preserved a high degree of crystallinity (95%) after exposure to liquid water at 190 °C, achieving a performance comparable to conventional micron-sized MFI crystals. These results demonstrate that controlled synthesis enables a systematic understanding of size-dependent properties in pure-silica MFI zeolites and that tungsten-assisted stabilization is an effective strategy to produce water-tolerant nanosized MFI materials without compromising their structural advantages.

Agradecimentos/Acknowledgments

The authors are grateful for the financial support granted by the National Council for Scientific and Technological Development - CNPq (131517/2024-4) and the São Paulo Research Foundation - FAPESP, grant 2023/10544-0.

New Linker expansion route and metal-dependent gas adsorption in the IRMOF-74-III series

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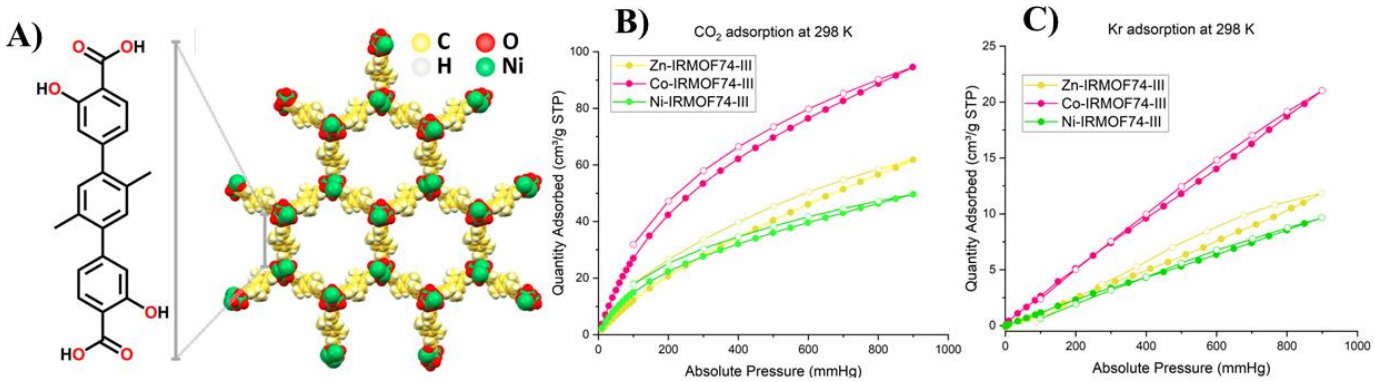
Palavras Chave:*MOFs,IRMOF-74-III,Suzuki–Miyaura coupling,Gas sorption,MOFs,IRMOF-74-III,Suzuki–Miyaura coupling,Gas sorption*

Highlights

M-IRMOF-74-III (M=Zn, Co or Ni) were obtained from**LINKER-III**synthesized via a new 4-step Suzuki–Miyaura coupling (60.2%). Co-IRMOF-74-III shows CO_2 uptake of 94.5cm^3g^{-1}, exceeding literature values.

Resumo/Abstract

Metal–organic frameworks (MOFs) are coordination networks built from metal nodes and organic linkers that generate accessible cavities that enable a wide range of applications. Here, we investigate the**IRMOF-74**series, isoreticular with**MOF-74**, characterized by one-dimensional hexagonal channels and systematic pore expansion through linker modification (Fig. 1a). To this end, 2,5-dihydroxyterephthalic acid was extended to a three-ring aromatic backbone through a new Suzuki–Miyaura coupling route, affording the extended linker**LINKER-III**(Fig. 1a) in four steps with a 60.2% overall yield, surpassing the five-step route (57% yield) reported by Deng et al. We also demonstrate the use of penicillin vials as miniaturized solvothermal reactors for optimizing the synthesis of**M-IRMOF-74-III**(M = Zn, Co or Ni), reducing reagent consumption. The effect of the metal-salt counterion on MOF synthesis was evaluated: acetate maximized material yield, whereas chloride increased the crystallinity for**Co-IRMOF-74-III**. Adsorption/desorption isotherms of CO_2 (298 K, Fig. 1b), H_2 (77 K), and Xe/Kr (298 K, Fig. 1c) show that the metal node identity governs gas-sorption performance within the M-IRMOF-74-III series. For CO_2,**Co-IRMOF-74-III**reaches 88.7 $cm^3\ g^{-1}$ (800 mmHg), exceeding the highest value reported for $–CH_2NH_2$ functionalized**Mg-IRMOF-74-III**(73.2 $cm^3\ g^{-1}$ at 800 mmHg), indicating that metal selection can rival linker functionalization strategies. This improvement is consistent with strengthened interactions at open metal sites (partially filled 3d orbitals), whereas for gases dominated by van der Waals interactions (H_2, Xe, and Kr), the behavior scales with accessible surface area and porosity. Moreover, we report for the first time Xe and Kr adsorption in the**IRMOF-74-III**family, broadening the application range of these adsorbents.**Zn-**and**Ni-IRMOF-74-III**exhibit lower gas uptake due to reduced accessible surface areas, most likely resulted from synthesis-induced defects.



A) LINKER-III and M-IRMOF-74-III structures; B) CO_2 and C) Kr adsorption isotherms of M-IRMOF-74-III

Agradecimentos/Acknowledgments

The authors are grateful to the funding agencies FAPEMIG, CNPq, and CAPES for financial support through research grants (APQ-05311-23, APQ-03469-25, and APQ-01948-22) and scholarships.

New phases of Shigaite-like layered double hydroxide with the compositions Ni6-xCuxAl3(OH)18][(SO4)2Na]·yH2O

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Palavras Chave:*Layered double hydroxides, Bimetallic, Trimetallic, Vegard's law,Layered double hydroxides,Bimetallic,Trimetallic,Vegard's law*

Highlights

Bimetallic and trimetallic shigaite-like layered double hydroxides (LDH) with the compositions $Ni_{6-x}Cu_xAl_3(OH)_{18}][(SO_4)_2Na]\cdot yH_2O$ were synthesized by co-precipitation at increased pH and characterized

Resumo/Abstract

Traditional or hydrotalcite layered double hydroxides (LDH) are represented by the formula $[M^{2+}_{1-x}M^{3+}_x(OH)_2](A^{n-})_{x/n}\cdot yH_2O$, where M^{2+} and M^{3+} correspond to the metals in the layer and $(A^{n-})_{x/n}\cdot yH_2O$ the intercalated anions. LDH intercalated with sulfate and alkali metals, with composition $[M^{2+}_6Al_3(OH)_{18}][(SO_4)_2Na]\cdot 12H_2O$, similar to the mineral Shigaite, have recently been synthesized. To expand these new class of compounds, bimetallic and trimetallic LDHs with composition $Ni_{6-x}Cu_xAl_3(OH)_{18}][(SO_4)_2Na]\cdot yH_2O$ (x= 0 to 6) were synthesized for the first time. For the synthesis of the compounds, solutions of the metals M^{2+}, Al^{3+} and Na_2SO_4, with different proportions between Ni^{2+} and Cu^{2+}, were titrated with a 1 mol L^{-1} NaOH solution to pH 8.0 under atmosphere of N_2. The materials were hydrothermally treated in an oven at 90 °C for 120 h, centrifuged at 4000 rpm, washed several times and dried at 60 °C for 72 h. The ICP-OES analyses confirmed that the compositions were very similar to the predicted ones and X-ray diffraction (XRD) patterns indicated that all materials exhibited a basal spacing close to 11 Å, typical of LDH intercalated with SO_4^{2-} in a double-layer arrangement, in the presence of hydrated Na^+. FTIR analyses showed bands attributed to the O-H bond, S-O bands of sulfate, in addition to a linear shifting of the M-O band due to the replacement of Ni by Cu, according with Vegard's law, which states that a linear correlation should be observed when metals with different ionic radii are used in a solid solution. A deviation from linearity was observed in the bimetallic phase containing only copper, due mainly to Jahn-Teller distortion effect. This study demonstrates that new trimetallic phases with potential new properties can be synthesized with different compositions and proportions of divalent metals in the presence of Al^{3+}, opening the possibility of applications in different areas.

Agradecimentos/Acknowledgments

This study was financed in part by the CNPq (F.W.: 303776/2023-4; A.R.S.: 172761/2023-9), CAPES and FINEP.

Novo componente ativo de protetores solares: Nitretos de carbono como alternativa segura aos óxidos metálicos

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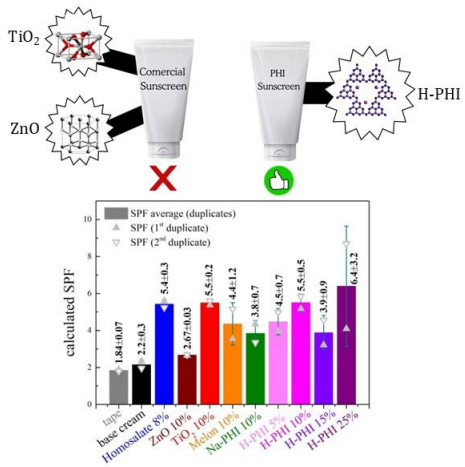
Palavras Chave:*Fator de proteção solar, método in vitro e livre de metais.,Método in vitro,Fator de proteção solar,Livre de metais*

Highlights

Crystalline protonated carbon nitride is a potential substitute to metal oxides used in sunscreens, offering comparable FPS and broader UV protection.

Resumo/Abstract

Filtros solares inorgânicos tradicionais podem ser prejudiciais à saúde devido à contaminação por metais tóxicos. Nitretos de carbono, em especial o poli(heptazina imida) protonado (H-PHI) que tem cor branca, podem ser uma alternativa uma vez que também são semicondutores inorgânicos. Neste trabalho, sintetizou-se o nitreto de carbono polimérico (PCN) via condensação térmica da melamina, a poli(heptazina imida) sódica (Na-PHI) pelo método de sal fundido (mistura de melamina e NaCl) e a H-PHI acidificando Na-PHI com HCl. Caracterizaram-se os materiais por ICP-OES, DRX, ATR-FTIR e MEV, confirmando sua estrutura típica e remoção eficiente de metais para obtenção de H-PHI. A formulação do protetor solar se deu pelo preparo de uma emulsão óleo em água, obtendo-se um creme contendo os componentes ativos. Prepararam-se protetores solares com os diferentes tipos de nitretos de carbono, TiO_2, ZnO e Homosalato, variando também a concentração. Para a avaliação*in vitro*da eficiência de proteção, aplicou-se cada protetor solar formulado a uma fita micropore, substrato que simula a pele. Mediu-se a transmitância em um espectrômetro de UV-Vis com o módulo da esfera integradora e calculou-se o Fator de Proteção Solar (FPS) na região UVB, o UVA-FPS e o comprimento de onda crítico (λc). Também se avaliou a fotoestabilidade das formulações ao expô-las à radiação de uma lâmpada de xenônio e a resistência à imersão em água. O H-PHI, particularmente na concentração de 10%, apresentou excelente absorção de radiação UV. Na região do UVB, o material possuiu uma performance similar aos óxidos metálicos, e na região do UVA a absorção da radiação é superior. Os resultados também indicaram que protetores solares com H-PHI são foto-estáveis e resistentes à imersão em água. Portanto, validou-se o H-PHI como um eficaz e promissor componente de filtro solar.



FPS calculado dos protetores solares formulados.

Agradecimentos/Acknowledgments

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OBTAINING LOW-COST ADSORBENTS USING COFFEE HUSK FOR ADSORPTION OF AZO DYES IN AQUEOUS MEDIUM

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Palavras Chave:*Agroindustrial waste,Azo dyes,Green chemistry,Water resources,Agroindustrial waste,Azo dyes,Green chemistry,Sustainability,Water resources*

Highlights

Low-cost adsorbents were successfully prepared. The materials were efficient in removing Crystal Violet Dye. Experimental data were best fitted by a Elovich model.

Resumo/Abstract

The use of agro-industrial waste for the production of low-cost adsorbents has gained prominence, given that they are generated in large quantities and have a high carbon content. In this context, coffee processing generates a large amount of husks, the improper disposal of which can cause serious environmental problems. In this study, coffee husks were used to obtain activated carbon (AC) and hydrochar (HC), which were subsequently supported with iron oxide and applied as adsorbents for the removal of crystal violet dye in aqueous medium. The materials were characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and point of zero charge (PZC) analysis. A solution containing 20 mg L^{-1} of crystal violet was used as a model contaminant. The kinetic study was performed using contact times from 10 to 180 min. The results of the kinetic study were investigated by applying pseudo-first-order, pseudo-second-order, and Elovich kinetic models. X-ray diffraction (XRD) analysis showed that the materials have an amorphous structure with disordered graphitic planes. In the FTIR spectrum, vibrational modes typical of carbonaceous materials were identified. The point of zero charge (PZC) was determined to be around pH 1-3, indicating that the material favors the adsorption of cationic species. The AC and HC materials removed 46% and 70% of the dye, respectively. Kinetic studies showed that the experimental data were well-fitted to the Elovich Model. suggesting that chemisorption is the predominant mechanism, combined with the effect of material surface heterogeneity. The results suggest that HC may constitute a low-cost and environmentally friendly alternative for the treatment of industrial effluents containing azo dyes. Thus, in addition to producing a low-cost adsorbent and adding value to the waste, the research also contributed to reducing the environmental impacts caused by the disposal of waste into the environment.

OBTAINING LOW-COST CATALYST FOR REMOVAL OF CRYSTAL VIOLET FROM AQUEOUS SOLUTION BY HETEROGENEOUS FENTON REACTION

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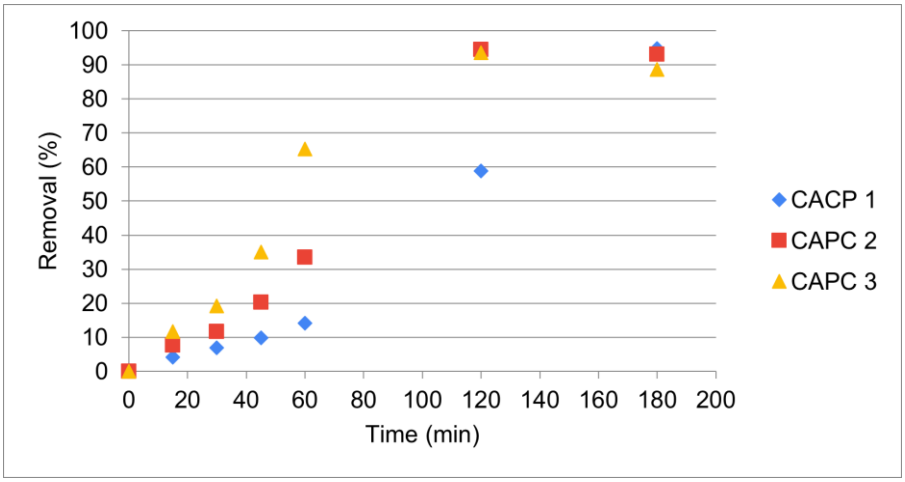
Palavras Chave:*Azo dyes,Coffee husks,Sustainability,Water resources*

Highlights

Low-cost catalyst was successfully prepared.
Catalyst was active in the removal of crystal violet dye by the heterogeneous Fenton reaction.
The kinetic data are better adjusted to first-order kinetics.

Resumo/Abstract

Fenton processes, based on the interaction between H_2O_2 and iron-based catalysts, are used to promote the formation of hydroxyl radicals (HO•). This process is simple and economical, not requiring sophisticated equipment. Heterogeneous Fenton reactions utilize solid catalysts, such as Fe_2O_3 and Fe_3O_4, which offer advantages in terms of efficiency and cost-effectiveness. This study aimed to prepare iron oxide supported on activated carbon produced from coffee husks and evaluate its efficiency in removing crystal violet dye through the heterogeneous Fenton reaction. The supported catalyst was produced by the incipient impregnation method and characterized by Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). For the catalytic tests, an aqueous solution of crystal violet dye was used as a model pollutant in the presence of the catalyst and with different aliquots of H_2O_2. The X-ray diffraction result showed the presence of hematite (α-Fe_2O_3) as the iron oxide phase in the produced material. It was observed that increasing the amount of peroxide promoted better decolorization rates in the initial stages of the kinetic study. However, after 180 minutes of reaction, it was found that experiments using 1 mL, 2 mL, and 3 mL of peroxide showed efficiency in removing approximately 95%, 93%, and 89% of the dye, respectively. The kinetic data of the catalysts were fitted to two kinetic models: first-order and second-order, in order to confirm these performances by comparing the values of the reaction rate constants. Comparing the correlation coefficients, it was found that the kinetic data better fit the first-order kinetics. According to the results obtained, it was observed that a low-cost material was produced with potential for application as a catalyst in advanced oxidation systems, expanding the possibilities of generating higher value-added products from agro-industrial waste.



Effect of the initial concentration of H2O2 in Heterogeneous Fenton Reaction

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Optimization of curcumin bioavailability using an albumin (BSA)-based controlled drug delivery system and green iron oxide (Fe3O4) nanoparticles

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Palavras Chave:*Curcumin,Albumin,Iron Oxide Nanoparticles,Green Chemistry,Drug Delivery*

Highlights

Green Fe_3O_4–BSA nanoparticles improve curcumin bioavailability.
A crosslinker-free system enables diffusion-controlled curcumin release for 5 days.

Resumo/Abstract

Problem: Curcumin comes from turmeric (*Curcuma longa*) and is antioxidant, anti-inflammatory, antitumor, antimicrobial and antiparasitic, has low cost and no side effects, making it a promising candidate for schistosomiasis mansoni treatment. However, curcumin is unstable and insoluble in water. Solution: Green iron oxide nanoparticles (Fe_3O_4-green NPs), a biocompatible carrier capable of interacting with magnetic fields, combined with bovine serum albumin (BSA), a biopolymer effective in encapsulating curcumin, have the potential to enhance its properties through a controlled release system. Objectives: This study aims to develop a controlled release system for curcumin encapsulated in BSA and carried by Fe_3O_4-green NPs. Methodology: Fe_3O_4-green NPs were synthesized following the principles of Green Chemistry, using Fe^{2+} ions, potato peel (Solanum tuberosum), and sodium carbonate. The system was produced using BSA in water, Fe_3O_4-green NPs, curcumin in ethanol, without a crosslinking agent. Characterization techniques included XRD, SEM, FTIR, TGA, DLS, UV/Vis, fluorescence, AGREE, and magnetic properties. Controlled release was conducted over 103 h (5 days) with 30 mg of the system and 2 mL of PBS, with 1 mL aliquots collected hourly and 1 mL PBS replenished. The concentration of released curcumin was determined via UV/Vis spectroscopy. Pharmacokinetics were analyzed using zero-order, first-order, Higuchi, Korsmeyer-Peppas, and Hixson-Crowell models, along with drug loading and encapsulation efficiency parameters. Results and Discussion: Functionalized Fe_3O_4-green NPs enabled a controlled, slow, and gradual release of curcumin over 103 h, reaching equilibrium at 1,8 g L-1. The Korsmeyer-Peppas model best fit the data, characteristic of diffusional polymeric systems. Conclusion: The produced system improved curcumin's properties, enhancing its bioavailability.

Agradecimentos/Acknowledgments

This work was supported by Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES).

Oxidized Lignin and Copper Oxide Nanorods Interactions: Investigation of Colloidal Stability and Ecotoxicity

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Palavras Chave:*Nanomaterials,Colloidal stability,Eco-corona,Ecotoxicology*

Highlights

- Oxidized lignin increases copper oxide nanorods colloidal stability

- Oxidized lignin causes minimal alterations to copper oxide nanorods ecotoxicity

Resumo/Abstract

Colloidal stability is critical for nanoparticles (NPs) behavior, as aggregation and precipitation affect their distribution and effective surface area, directly influencing its interaction with biological systems. While chemical functionalization strategies are commonly employed to enhance NP stability, the biomolecular corona formation has emerged as an alternative approach. Corona is the molecular layer spontaneously adsorbed on NP surface, influencing material's behavior. This work investigated the influence of oxidized lignin (OL) on the colloidal stability and ecotoxicology of copper oxide nanorods (CuONR). Structural characterization confirmed that the CuONR exhibits a monoclinic CuO crystal structure with an average length of 31 nm and width of 6 nm. Upon interaction with OL, the ζ-potential shifted from +33 mv to -49 mV, indicating corona formation. CuONR suspension rapidly precipitated in reconstituted water media while the OL promoted its stabilization for more than 48h, indicating the effect of OL on CuONR colloidal stability. Aggregation kinetics experiments revealed significant increase in the critical coagulation concentration, from 7 mM to 159 mM NaCl. This increase was consistent with DLVO theory and supported by theoretical predictions. The impact on the CuONR ecotoxicity was evaluated using multiple model systems. Minimum inhibitory concentration assays against*Bacillus subtilis*showed no significant differences between CuONR with or without corona formation. Similarly, acute toxicity assays with*Danphnia similis*revealed comparable EC_{50} values for both conditions. Germination assays with*Solanum lycopersicum*L. indicated lower seedling development at elevated concentrations (≥1.5 mg/L) for CuONR+OL. Overall, OL is an effective biopolymer to increase colloidal stability of CuONR minimally affection CuONR ecotoxicity, highlighting OL as a promising sustainable stabilizing agent for engineered nanomaterials, with reduced environmental impacts.

Agradecimentos/Acknowledgments

This project was developed at LNNano/CNPEM

Oxygen vacancy stability in CeO2 and Pd/CeO2 systems

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Palavras Chave:*CeO2 surface; oxygen vacancy,DFT periodic calculations,CeO2 surface,oxygen vacancy*

Highlights

The stability of oxygen vacancies in CeO_2 and Pd/CeO_2 systems enables us to assess the extent to which this surface supports catalytic processes, including the hydrogenation of CO_2.

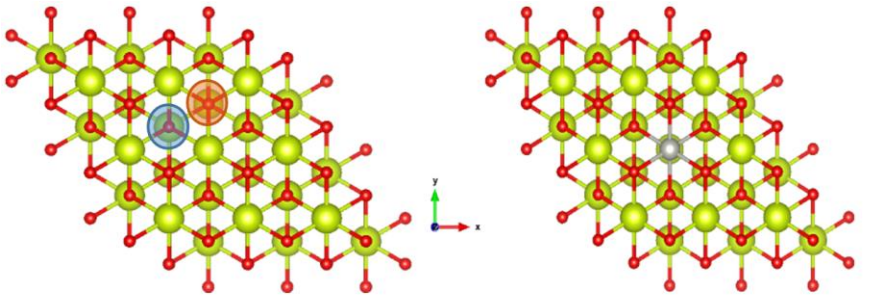
Resumo/Abstract

All DFT calculations were performed using the QUICKSTEP code of the CP2K package (v. 2025.2)[1]. Exchange–correlation was calculated with the PBE generalized gradient approximation (GGA), GTH pseudopotentials, and MOLOPT basis sets (triple-ζ for Ce and double-ζ for O), including D3 dispersion corrections. To properly describe reduced ceria containing oxygen vacancies and Ce^{3+} centers, we employed DFT+U for all Ce 4f states (Mulliken-population-based), using $U_e$ff = 7.0 eV to reproduce experimental band gaps and work function results[2]. We studied the stability of oxygen vacancies in CeO_2 slab and in Pd/CeO_2 systems, in which a Pd atom replaced a Ce atom. For example, removing an oxygen atom from the CeO_2 (111) surface, leaves excess electrons that tend to localize on neighboring cerium cations (partial reduction $Ce^{+4} \rightarrow Ce^{3+}$), increasing the Fermi level and decreasing the work function[3] (Φ, the minimum energy required to remove an electron from the material to vacuum), from 4.77 to 4.00 eV, and decreasing the band gap from 3.12 to 2.75 eV. We analyzed energy differences, charge redistribution, and related electronic/structural properties for multiple oxygen-vacancy configurations in both systems. Understanding how these vacancies form and behave is relevant to the initial steps of CO_2 hydrogenation to methanol. Unpublished experimental data support this approach.

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[3] Lin, L. et al. Work Function: Fundamentals, Measurement, Calculation, Engineering, and Applications. Phys. Rev. Applied 2023, 19, 037001.



CeO_2(111) - the oxygen atom marked by the blue circle corresponds to the most external (surface) site, and the one marked by the red circle represents a more internal (subsurface) site (left). Pd substitution is obtained by replacing a single Ce atom with Pd (right).

CeO_2(111)

Agradecimentos/Acknowledgments

The authors acknowledge CAPES and FAPESP (grants 2024/10909-0, 2025/19394-6).

Perovskite phase formation in $LaMnO_3$ synthesized by the microwave-assisted hydrothermal (MAH) method

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Palavras Chave:*Perovskite materials,Microwave-assisted hydrothermal synthesis,LaMnO3,Rare earth oxides*

Highlights

$LaMnO_3$ was synthesized by the MAH method.
Perovskite phase formation suggests suitability for gas sensing applications.

Resumo/Abstract

Perovskite-type oxides have attracted increasing attention in materials science due to their structural versatility and potential functional applications. Among them, lanthanum manganite ($LaMnO_3$) is a p-type semiconductor with promising electrical and catalytic properties, making it a candidate material for gas sensing applications. In this work, $LaMnO_3$ was synthesized by the microwave-assisted hydrothermal (MAH) method aiming to investigate the formation of the perovskite phase and discuss its potential use as a functional material.

The obtained material was characterized by X-ray diffraction (XRD) to evaluate phase formation and structural features. The diffraction pattern confirmed the formation of the $LaMnO_3$ perovskite phase, indicating that the MAH method is suitable for obtaining phase-pure materials under the studied conditions.

These results demonstrate that the MAH route is a promising and efficient approach for the synthesis of $LaMnO_3$ with perovskite structure, motivating future studies focused on microstructural control and evaluation of its performance in gas sensing applications.

Agradecimentos/Acknowledgments

This work was supported by CAPES – Finance Code 001. The authors also acknowledge CNPq for grant 311453/2021-0, as well as to FAPESP, which provided grants #2022/05381-1, #2022/14720-4, #2020/02471-4, #2020/06421-1, and #2024/03388-4.

Photo- and sonochemistry activation of a hybrid TiO_2/porphyrin composite for thionine dye degradation

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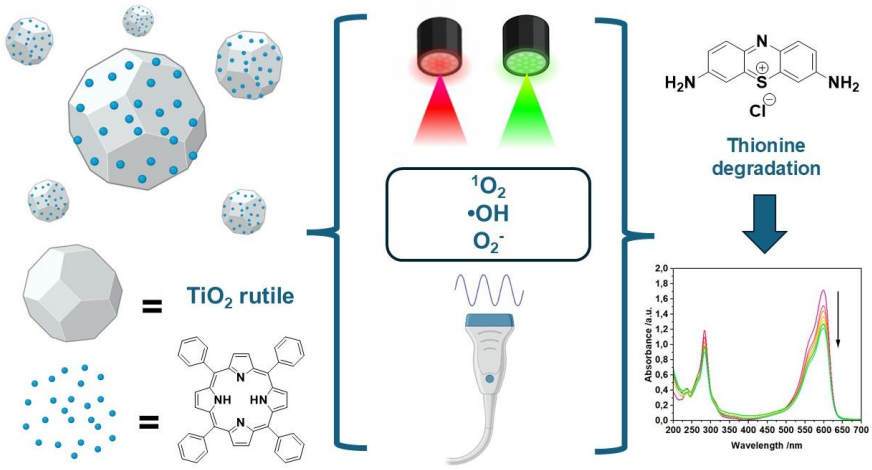
Palavras Chave:*photochemistry,degradation of dyes,sonochemistry,porphyrin*

Highlights

A hybrid composite (H_2TPP/TiO_2) was synthesized and characterized. Photo- and sonochemistry produced reactive oxygen species. Thionine degradation kinetics were calculated.

Resumo/Abstract

Oxidative processes involving light and a photosensitizer have long been studied, and more recently the use of acoustic waves in the ultrasound frequency range (>20kHz) has also been proposed as a strategy for generating reactive oxygen species (ROS). The degradation of dyes represents a robust and informative approach for investigating these phenomena. This study showcases the synthesis and characterization of a hybrid composite based in tetraphenylporphyrin (H_2TPP) and rutile titanium oxide (TiO_2), and its application as a photo- and sonosensitizer for the degradation of thionine. Diffuse reflectance and FT-IR spectroscopy confirm the optical H_2TPP properties of the composite, while SEM imaging and XRD patterns reveal a rod-shaped, porous rutile material. ASAP analysis shows that the surface area and pore volume of H_2TPP/TiO_2 are lower than those of TiO_2, consistent with porphyrin adsorption. Photobleaching experiments demonstrate that green LED irradiation is more effective than red LED light, leading to up to 45% thionine degradation during 80 minutes of light exposure. Leucothionine, a fluorescent degradation product, was detected during photobleaching but was not observed under ultrasound irradiation. Under ultrasound conditions (1MHz, 1W cm^{-2}), the composite promoted approximately 40% thionine degradation within 30 minutes, whereas a pure thionine solution showed roughly 15% degradation, indicating that H_2TPP/TiO_2 enhances ROS generation via water sonolysis.



Composit H2TPP/TiO2 and its application as photo- and sonosensitizer to generate ROS

Agradecimentos/Acknowledgments

The authors acknowledge CNPq (Grant 141771/2025-9), Fapesp (Grant 2025/09760-5) and RELAM-UFU.

Photocatalytic nanocomposites based on g-C3N4 and SiO2/TiO2 aerogels for enhanced photodegradation of aqueous dyes.

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Palavras Chave:*g-C3N4,aerogel,silica,photocatalysis*

Highlights

This work describes the solid-state synthesis of the g-C3N4 nanocomposite at different concentrations, as well as its structural properties.

Resumo/Abstract

Environmental pollution has been one of the biggest environmental problems in modern society. Therefore, heterogeneous photocatalysis has stood out as a sustainable and efficient technology for treating environmental pollutants. Among visible photocatalysts, graphitic carbon nitride (g-C_3N_4) stands out as one of the most promising photocatalysts for applications under visible light; it is a metal-free, stable material with good light absorption in the visible region. Although g-C_3N_4 stands out as one of the most promising photocatalysts for visible light applications, its performance is still limited by some structural properties and electronic lights (low adsorption capacity and limited concentration in the UV region). Therefore, this work consists of incorporating silica and/or titanium oxide-composed aerogels into g-C_3N_4 to form a nanocomposite (g-C_3N_4/SiO_2 -TiO_2) with high photocatalytic efficiency. The hypothesis is that the presence of silica aerogel should increase the surface area and, consequently, the adsorption capacity of the nanocomposite, while TiO_2 can extend its photocatalytic efficiency to the UV region, enabling the absorption of both UV and visible light. The aim of this study is to evaluate the efficiency of the nanocomposite (g-C_3N_4/SiO_2 -TiO_2) in the absence and presence of SiO_2 and/or SiO_2 -TiO_2 aerogel, using a photocatalytic assay with RhB (rhodamine B) dye as a pollutant model. Furthermore, the work involves structural characterization, analyzing the crystallinity of the material through X-ray Diffraction (XRD) and morphological analysis of the nanocomposite using Scanning Electron Microscopy (SEM). The work is in its initial phases; therefore, so far, solid-state synthesis, photocatalytic testing (showing complete administration of the RhB dye (10 ppm) in just 35 minutes, and XRD analysis have been performed, which showed that the nanocomposite consists of g-C_3N_4 and TiO_2 in rutile and anatase phases.

Agradecimentos/Acknowledgments

This work was supported by CAPES, CNPq, FAPESP, and USP.

Photocurable Glycerol-Maleic Anhydride Resins: Renewable and Shape-Memory polymer 3D Printing

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Palavras Chave:*3D printing, glycerol, renewable polymers, smart polymers*

Highlights

Production of a shape-memory material from a renewable and photocurable resin derived from glycerol and maleic anhydride

Resumo/Abstract

Additive manufacturing, particularly vat photopolymerization (VP) 3D printing, enables the rapid fabrication of high-resolution rigid or flexible objects through light-induced polymerization of liquid resins. Beyond complex geometries, VP is a promising route for producing smart polymers capable of responding to external stimuli such as temperature, stress, pH, or light. However, most smart polymer monomers are derived from fossil resources, raising sustainability concerns and highlighting the need for renewable alternatives. Despite this demand, the diversity of renewable feedstocks explored for VP remains limited. In this context, a polyester containing polymerizable C=C bonds derived from glycerol and maleic anhydride (PPH) emerges as a promising renewable feedstock for vat photopolymerization. In this work, three photocurable resins were formulated using PPH, 2-hydroxyethyl methacrylate (HEMA), and diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide (TPO) as photoinitiator. The TPO content was fixed at 3 wt.%, while the PPH/HEMA ratios were 30/70 (PPH30), 50/50 (PPH50), and 70/30 (PPH70). The resulting materials (POL30, POL50, and POL70) were printed under previously reported conditions and post-cured under UV irradiation for 2 h. Thermal and thermomechanical properties were evaluated by TG/DTG-DTA and DMA. Thermal stability temperatures of 134.7, 127.5, and 120.7 °C were obtained for PPH50, PPH70, and PPH30-based materials, respectively, with similar degradation profiles showing three main mass-loss steps. Glass transition temperatures were 56.5, 54.1, and 16.0 °C for POL30, POL50, and POL70, respectively, and secondary β-transitions were observed due to semi-interpenetrating polymer networks. Shape-memory tests on POL30 revealed high shape-fixity (>94%) and an increase in shape-recovery from 70% to 91% over successive cycles. These results highlight the potential of renewable polyesters for VP-based additive manufacturing of smart materials.

Agradecimentos/Acknowledgments

FAPESP (grant: 2024/14279-1; 2024/00779-2; 2025/12505-7; 167096/2025-7), CNPq (grant 303968/2024-9), CAPES (grant 88887.146236/2025-00).

PLA/Graphite Conductive Filaments: The Role of Surfactants in the Electrochemical Performance of 3DPrinted Sensors

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Palavras Chave:*3D printing,Electrochemical sensors,Surfactants,Graphite dispersion,Conductive filaments*

Highlights

Development of PLA/graphite conductive filaments for 3D-printed electrochemical sensors.

Evaluation of surfactants as dispersion agents for graphite in polymeric matrices.

Resumo/Abstract

Conductive filaments have gained prominence in the context of additive manufacturing, especially for applications in electrochemical sensors. However, commercially available formulations still face limitations, such as low electrical conductivity and the need for surface treatments, which restrict their direct use in functional devices. Thus, the development of new filaments that combine good conductivity, flexibility, and printability is essential for advancing this field.

This work aimed to develop, characterize, and compare conductive filaments based on polylactic acid (PLA), graphite, and castor oil, evaluating the effect of different dispersion strategies of conductive particles on material homogeneity and the electrochemical performance of 3D-printed sensors. The filaments were formulated with approximately 40 wt.% graphite and castor oil contents ranging from 5 to 10 wt.% as a plasticizer, varying according to the formulation and the presence of surfactants, with PLA as the polymeric matrix, and processed by extrusion under controlled temperatures.

Given that the efficiency of conductive particle dispersion directly influences the electrical and mechanical properties of the filament, the effects of adding surfactants—sodium dodecyl sulfate (SDS), cetyltrimethylammonium bromide (CTAB), and polysorbate 80 (Tween 80)—were investigated at approximately 5 to 10 wt.% relative to the conductive fraction. Filaments produced without surfactants exhibited good flexibility, excellent printability, and thermal stability up to ~330 °C, as evidenced by thermogravimetric analysis (TGA). Electrochemical tests in 5 mM $K_4[Fe(CN)_6]$ solution with 0.1 mM KCl indicated that SDS and CTAB did not significantly enhance sensor performance. New formulations containing Tween 80 are currently under evaluation, aiming to optimize graphite dispersion and improve the electrochemical performance of the sensors, with potential applications including pesticide detection.

Agradecimentos/Acknowledgments

The authors acknowledge FAPERJ for the technological initiation scholarship (E-26.260.058/2025), as well as FAPERJ (E-26/290.009/2023) and CNPq (406419/2021-3 and 408001/2023-2) for financial support.

Polymeric nanoparticulated hydrogel containing S-nitrosoglutathione for biomedical applications

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Palavras Chave:*Nitric oxide donor,Chitosan nanoparticles,Alginate matrix,Biodegradable platform,Sustained release.*

Highlights

Biodegradable alginate–chitosan hydrogel platform for sustained and tunable nitric oxide delivery

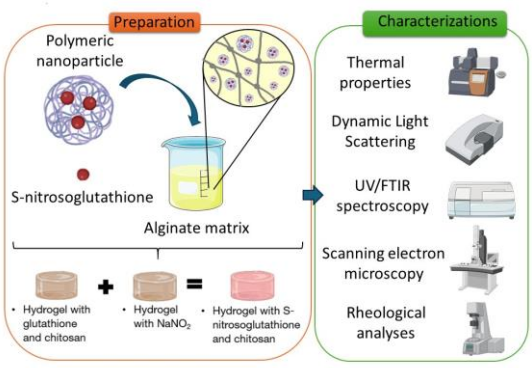
Resumo/Abstract

Glutathione is a tripeptide capable of undergoing nitrosation in an acidic environment, forming S-nitrosoglutathione, a low molecular weight molecule used here as a nitric oxide donor. Nitric oxide is an endogenous free radical that plays several fundamental physiological and pathophysiological roles, such as vasodilation, tissue repair, tumor modulation, cell communication, and antimicrobial defense.

In this work, glutathione was encapsulated into chitosan nanoparticles, which were then dispersed within an alginate hydrogel. An*in situ*nitrosation process was proposed by mixing hydrogels with different pH values, resulting in the*in situ*formation of S-nitrosoglutathione and the spontaneous release of nitric oxide. The obtained chitosan nanoparticles exhibited a positive charge and a size below 90 nm, being dispersed in an alginate matrix crosslinked with calcium via the ionotropic gelation method.

The three-dimensional structure was characterized by spectroscopic and thermogravimetric techniques. Rheological analysis revealed a shear-thinning behavior, with the storage modulus (G') exceeding the loss modulus (G') within the linear viscoelastic region. The*in situ*formation of S-nitrosoglutathione was monitored by UV-Vis spectroscopy, and its decomposition kinetics were tracked, demonstrating a sustained release of nitric oxide for at least 3 days. Diffusion analysis showed that the system follows the Higuchi kinetic model, governed by the classic Fickian diffusion mechanism of S-nitrosoglutathione.

Electrochemical quantification confirmed the release of nitric oxide at bioactive concentrations (approximately 25 µmol $NO \cdot g^{-1}$). Cytotoxicity assays in HaCaT keratinocytes showed that the hydrogel is cytocompatible at concentrations of clinical interest. This resulted in a stable, non-cytotoxic, and multifunctional hybrid platform that offers sustained and modulated nitric oxide release.



Preparation and characterization of S-nitrosoglutathione loaded biodegradable hydrogels

Agradecimentos/Acknowledgments

We are thankful for the financial support from Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES), CNPq, São Paulo Research Foundation (Fapesp), and INCT Nanotechnology for Sustainable Agriculture.

Pontos de carbono ternários multifuncionais na agricultura óptica: avaliação dos efeitos biométricos e metabólicos em culturas de pitanga

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Palavras Chave:*Nanofertilizantes, Carbon dots, dopamento químico, fotossíntese, nutrição vegetal*

Highlights

O uso de pontos de carbono dopados com boro, silício e nitrogênio favoreceu o crescimento vegetal e apresentou efeito elicitor na produção de curzereno (metabólitos antioxidantes e anti-inflamatório).

Resumo/Abstract

O Brasil é um dos principais produtores agrícolas do mundo, mas, ainda em 2025, depende do abastecimento de fertilizantes e defensores agrícolas estrangeiros. Por esse motivo, vem se buscando novas alternativas de adubos e defensores nacionais. Nesse contexto, os pontos de carbono (PC) vêm ganhando maior visibilidade no que tange o aprimoramento da produção agrícola. Sendo assim, o objetivo deste trabalho é sintetizar um PC dopado com nitrogênio, boro e silício (BNSi-PC) e avaliar seus efeitos na cultura da pitanga vermelha (*Eugenia uniflora*). Parâmetros biométricos, quantificação de compostos voláteis e correlação com vias metabólicas do vegetal; (3) avaliação do efeito induzido sobre o processo fotossintéticos, no fortalecimento da parede celular vegetal e nível de nutrição da planta. A síntese dos BNSi-PC foi realizada por rota hidrotermal. A caracterização dos BNSi-PC foi realizada por meio de espectroscopias de luminescência, de absorção eletrônica, vibracional e de energia dispersiva. As morfologias das nanopartículas foram analisadas por microscopia eletrônica de varredura. O perfil de voláteis e a composição do óleo essencial foram analisados em um cromatógrafo gasoso acoplado à espectrometria de massas. A formação dos BNSi-PC foi evidenciada pelos sinais característicos das técnicas mencionadas, especialmente na EDD. O método*headspace*confirmou a presença de diversos semioquímicos importantes, além da elevação de >250% no teor de curzereno. Também foi observado o efeito das nanopartículas na ativação e desativação de rotas biológicas de síntese de substâncias associada a comunicação com agentes polinizadores. Os resultados biométricos obtidos com a aplicação dos BNSi-PC indicaram aumento em todos os parâmetros avaliados.

Agradecimentos/Acknowledgments

Aos órgãos de fomento CAPES, CNPq e FACEPE. À Universidade Federal Rural de Pernambuco e o Laboratório de Medicamentos, Tecnologias, Energia e Soluções Ambientais (LaMTESA/UFRPE).

Porous Au/Ag Alloy-Shell Au Nanorods as Plasmonic Nanoresonators for High-Performance SERS Platforms

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Palavras Chave:*Plasmonic nanoresonators,Core-shell nanostructures,Surface-Enhanced Raman Scattering (SERS)*

Highlights

Plasmonic nanoresonators were developed as active SERS substrates; Comparative study of Au–Ag core–shell nanorod nanostructures; Rhodamine 6G detection used to evaluate SERS performance.

Resumo/Abstract

Surface Enhanced Raman Scattering (SERS) relies on the amplification of the Raman signal arising from the collective excitation of conduction electrons at nanostructured metallic surfaces.This excitation generates intense localized electromagnetic fields associated with the oscillation of delocalized electrons at the metal–molecule interface.The resulting electromagnetic field enhancement increases the effective polarizability of adsorbed molecules, giving rise to strongly enhanced Raman scattering and enabling ultrasensitive molecular detection.In this context,gold nanorods were synthesized following the method by Xu et al and modified through silver shell deposition and a controlled galvanic replacement reaction,leading to a core–shell nanostructure consisting of a gold nanorod core coated with a porous Au–Ag alloy shell.These plasmonic nanoresonators are capable of promoting plasmonic coupling between adjacent nanofeatures,resulting in the formation of electromagnetic hot spots and enhanced SERS sensitivity.AuNRs were initially characterized by UV–Vis spectroscopy,exhibiting localized surface plasmon resonance bands centered at 525nm and 759nm,corresponding to the transverse and longitudinal modes,respectively.The STEM revealed average dimensions of 46nm in length and 18nm in width.After silver shell deposition,Au@AgNRs displayed LSPR bands shifted to 504nm and 665nm,reflecting the Ag coating.Subsequent galvanic replacement led to porous nanostructures,with LSPR bands shifting back toward those of the pristine AuNRs,at 521nm and 760nm.The nanostructures were comparatively evaluated as active SERS substrates using the drop-casting method with rhodamine 6G as a probe molecule.Preliminary results revealed an average SERS intensity of 18956 counts for the band at 613.6 cm^{-1}, attributed to the in-plane bending mode of the aromatic ring of R6G.Following optimization of acquisition parameters,the SERS activity of substrates of Au@AgNRs and Au@hAuAgNRs will be evaluated.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from FAPESP (2025/23131-0) and CNPq (306073/2024-2, 444106/2024-3), and thank LNNano-CNPEM and LISpec (RRID: SCR_027391/CEMUIQ-UNICAMP) for technical support.

Preparation and characterization of biodegradable starch/cellulose blends via cold alkaline dissolution and ethanol-induced precipitation

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Palavras Chave:*Polymeric blends,Cellulose,Corn starch,Alkaline solution,Co-precipitation.*

Highlights

Biodegradable starch/cellulose blends prepared via cold NaOH dissolution.

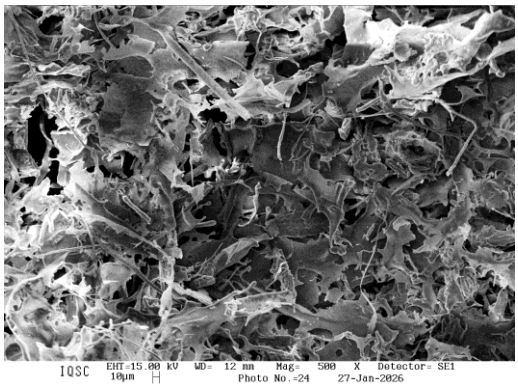
Ethanol addition promotes simultaneous precipitation and improved homogeneity.

Resumo/Abstract

The development of biodegradable materials from abundant natural polymers, such as starch and cellulose, is essential for sustainable alternatives to synthetic plastics. Despite their chemical similarities, structural differences and distinct solubility profiles make the joint processing of these polysaccharides challenging. This work describes the preparation of polymeric blends of corn starch (CS) and microcrystalline cellulose (MCC) using a cold alkaline dissolution system (NaOH) to produce materials with distinct morphological properties.

The methodology involved the dissolution of CS and MCC (1:1 ratio) in a cold NaOH solution, carefully controlled to prevent premature starch gelatinization. For polymer regeneration, dialysis against distilled water was performed until neutralization. Two precipitation methods were compared: direct dialysis (sample 1S1C.1) and the addition of ethanol to the alkaline solution prior to dialysis (sample 1S1C.2) to induce simultaneous co-precipitation. Isolated samples (processed MCC and CS, labeled 0S1C and 1S0C) were used as controls. The resulting materials were freeze-dried, yielding white, cotton-like fibers.

The samples were characterized by FTIR, XRD, and SEM. FTIR spectra confirmed the preservation of functional groups across all samples. XRD analysis revealed that cellulose-containing samples (0S1C, 1S1C.1, and 1S1C.2) underwent a transition from cellulose I to cellulose II after regeneration, while the isolated starch (1S0C) exhibited a predominantly amorphous structure. SEM results provided the most significant findings: sample 0S1C displayed a fibrous morphology, whereas 1S0C appeared as thin sheets. The 1S1C.1 blend showed a heterogeneous mixture of both phases. In contrast, sample 1S1C.2 (with ethanol) presented a more homogeneous microstructure, distinct from its precursors, confirming that ethanol enhances the interaction between polysaccharides during precipitation.



SEM micrograph of the 1S1C.2 starch/cellulose blend

Agradecimentos/Acknowledgments

The authors thank the Physical Organic Chemistry Group (IQSC-USP) for the technical support and the National Council for Scientific and Technological Development (CNPq) for the financial support and research fellowships.

Pressure-sensitive conductive hydroxypropyl methylcellulose and nickel(II)hexacyanoferrate(II) composite cryogel

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Palavras Chave:*Cryogel, Prussian blue analog, electric resistivity, hydroxypropyl methylcellulose, pressure-sensitive.*

Highlights

Novel composite cryogels of HPMC and NiHCF.
The electrical resistivity of the composite cryogels was significantly lower than that of pure HPMC cryogels, and decreased with compression.

Resumo/Abstract

The search for renewable-source materials with variable electrical resistivity is relevant in the current scenario in applications such as wearable devices and piezoresistive sensors. In this work, composite cryogels of hydroxypropyl methylcellulose (HPMC) and Prussian blue analog (PBA) nickel(II) hexacyanoferrate(II) (NiHCF) were developed, and their electrical resistivity was evaluated as a function of compression. NiHCF particles were synthesized by coprecipitation directly in an aqueous solution of HPMC (30 g/L) by mixing iron hexacyanoferrate(II) and nickel chloride at 24 °C under magnetic stirring for four hours. After this period, the dispersion was molded, frozen and lyophilized, generating composite cryogels. The scanning electron microscopy image in Figure 1 shows typical cubic NiHCF particles distributed on the HPMC porous walls. The electrical resistivity of the cryogels was measured using a Keithley 2420 SourceMeter multimeter while compressed in an IP90DI dynamometer. The electrical resistivity of the composite cryogels decreased from 2 MΩto 0.2 MΩwhen the compression was 20%. This value did not change significantly for higher compressions. Pure HPMC cryogels did not show a decrease in electrical resistivity under compression. This resistivity decrease is consistent with compression-induced densification of the porous network, which increases the number of conductive contacts among NiHCF particles and reduces interparticle contact resistance, facilitating charge transport through a more continuous percolation pathway.These preliminary results indicate the potential application of HPMC/PBA hybrid cryogels as pressure-sensitive conductive materials.

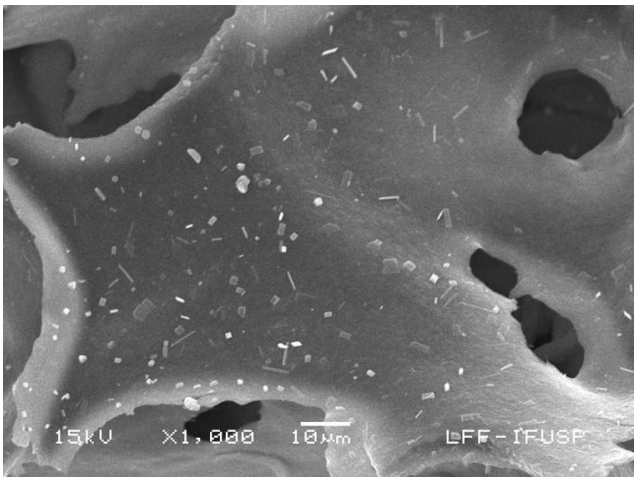


Figure 1. Scanning electron microscopy of HPMC/NiHCF cryogel

Agradecimentos/Acknowledgments

The authors acknowledge FAPESP (Grants 2024/20008-0 and 2024/19156-5) and CNPq (Grant 304017/2021)

Probing thermal and SiO2 shell effects on optical response of YF3:Eu3+ using synchrotron light

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Palavras Chave:*YF_3:Eu^{3+},SiO_2 shell,structural and morphological behavior,XEOL*

Highlights

Microwave-assisted synthesis is reliable to produce YF_3:Eu^{3+} particles; Thermal treatment and SiO_2 shell drive structural and morphological reorganization; Eu^{3+} symmetry in YF_3:Eu^{3+}@SiO_2

Resumo/Abstract

YF_3:Eu^{3+} particles were synthesized via a microwave-assisted hydrothermal route, yielding highly crystalline materials with controlled morphology. Amorphous SiO_2 shells were deposited by the Stöber method, producing YF_3:Eu^{3+}@SiO_2 core–shell systems investigated before (AP) and after thermal treatment (TT) at 400°C/4h. Structural and spectroscopic characterizations confirmed the orthorhombic YF_3 phase, Eu incorporation, and the formation of thin silica shells on YF_3:Eu submicrometric particles. Synchrotron-based techniques such X-ray absorption near-edge structure (XANES) and X-ray excited optical luminescence (XEOL) confirmed the presence of Eu in the 3+ state and the characteristic Eu^{3+} $^5D_0$ --> ^7F_n (n = 0, 1, 2, 3, 4) transitions. PL and XEOL emission spectra are dominated by $^5D_0$ --> $^7F_1$ transition, indicating Eu^{3+} ions are in high-symmetry sites. For YF_3:Eu^{3+}@SiO_2-TT, a decrease on the ratio $^5D_0$ --> $^7F_2$/ $^5D_0$ --> $^7F_1$ suggests Eu^{3+} are in higher symmetry sites. This behavior is in accordance with structural changes observed by XRD through an increase in the ratio [1 1 1]/[0 2 0], and with a morphological evolution, observed by SEM, from rod-like (530 nm x 230 nm) in YF_3:Eu and AP to more spherical (~360 nm) particles in TT samples. TEM micrographs reveal that the particles are composed of clusters with subunits ranging from 20 – 30 nm, which might be associated with growth in different crystalline orientations. The presence of SiO_2 in both AP and TT samples is further confirmed by FTIR, EDS, and XPS analyses. Raman spectra exhibit a shift from 400 to 404 cm^{-1}, suggesting the presence of compressive strain induced by the SiO_2 shell. Then, combined structural, morphological, and spectroscopic results demonstrate that the SiO_2 shell and subsequent thermal treatment promote important rearrangements in YF_3:Eu^{3+} particles, leading to an increase in the local symmetry around Eu^{3+} ions and in its optical response under UV and X-rays irradiation as observed in Figure 1.

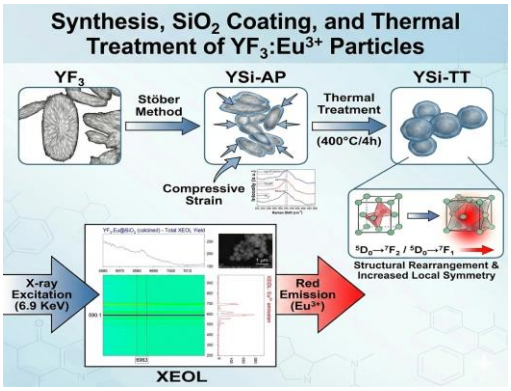


Figure 1. General description of main results

Agradecimentos/Acknowledgments

This work was developed at LPCM and CMNano/UFS, IQ/USP, LNNano and LNLS/CNPEM; and was financially supported by AGITTE (25/2024), CNPq, FINEP, FAPITEC and FAPESP (2021/08111-02)

Produção de biopolímeros como alternativa sustentável para a indústria da moda

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Palavras Chave:*Biopolímeros, Indústria Têxtil, Amido, Sustentabilidade, Química Verde.,Biopolímeros,Indústria Têxtil,Amido,Sustentabilidade,Química Verde*

Highlights

The silent pollution caused by the fashion industry

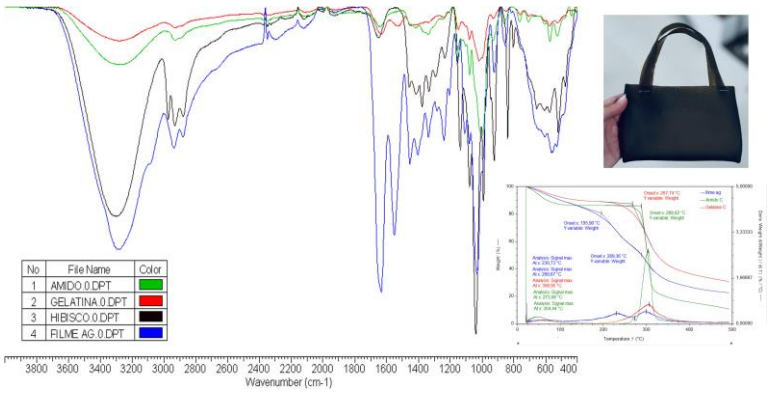
Synthesis of biopolymer from starch and gelatin

Application of biopolymer in the textile industry

Resumo/Abstract

A indústria da moda é uma das mais poluentes do mundo, movimentando trilhões de dólares anualmente sob dependência crítica de polímeros sintéticos derivados do petróleo, como o poliéster[1], poliamida[2] e o policloreto de vinila (PVC)[3]. O descarte e a lavagem desses materiais agrava a crise global de microplásticos e emissões de gases de efeito estufa (GEE)[2]. Este trabalho apresenta a síntese de um biopolímero criando uma alternativa esteticamente viável e ambientalmente responsável para o setor têxtil. O biopolímero foi produzido a partir de amido e gelatina, utilizando óleos naturais como conservante e antifúngico. A produção do biopolímero baseou-se na gelatinização do amido de milho reforçado com gelatina, sob hidrólise parcial ácida (ácido acético) para redução das ramificações da amilopectina. Foram realizados testes de otimização da composição variando os plastificantes utilizados (glicerol, sorbitol e PG) e concentrações de aditivos para melhorar resistência mecânica e biológica. O produto final foi obtido a partir de 80 mL de H_2O, 56 g de gelatina, 4 gotas de óleo essencial de canela, 7 mL de ácido acético (4%), 10,5 g de amido e 35 mL de extrato de hibisco em propilenoglicol, apresentando assim, o melhor equilíbrio entre flexibilidade e durabilidade. O PG mostrou-se superior aos demais plastificantes na integração com o corante natural. As análises de Infravermelho por transformada de Fourier e análises termogravimétricas evidenciam a modificação estrutural do biopolímero em relação aos materiais de partida. O produto final demonstrou viabilidade para produção em escala (peças de 25x32 cm), apresentando secagem natural em 5 dias sem proliferação microbiana, culminando na confecção de um protótipo funcional (bolsa).

1) SMELIK, A. Fashion Practice, 15, 279 - 299, 2023. 2) SOARES, H. M. S. et al. Revista Interdisciplinar Científica Aplicada, 19, 33-65, 2025. 3) PIATTI, T. M. Plásticos: características, usos, produção e impactos ambientais - Maceió: EDUFAL, 2005.



Análises de IVTR e ATG do biopolímero modificado e foto de sua aplicação

Agradecimentos/Acknowledgments

Os autores são gratos pela infraestrutura do Centro Multiusuário do Centro de Ciências Tecnológicas da Universidade do Estado de Santa Catarina (CMU/CCT/UDESC) e a infraestrutura do Sesi Referência Joinville pelo laboratório e reagentes utilizados.

Production of carbon felt based electrodes modified with transition metal dichalcogenides for Hydrogen Evolution Reaction (HER)

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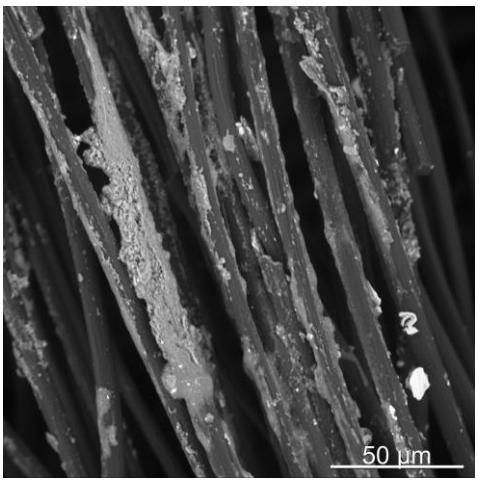
Palavras Chave:*Hydrogen,Carbon Felt,Synthesis,TMD,Molybdenum Disulfide*

Highlights

The direct synthesis of MoS2 on the surface of carbon felt using a bnider-free methodology led to a electrode with Pt-like behavior.

Resumo/Abstract

In view of the economic challenges associated with the use of noble metal electrocatalysts for the hydrogen evolution reaction (HER), investigating alternative pathways to reduce sustainable energy production costs is mandatory. Molybdenum Disulfide (MoS_2) stands out as one of the most promising substitute materials due to its optoelectronic properties and chemical stability. Similar to Platinum, the edge sites of MoS_2 possess a hydrogen adsorption free energy close to zero, revealing a favorable environment for HER. However, the intrinsic electrocatalytic activity of MoS_2 is limited to edges and defects, while its basal plane remains thermodynamically inert. Therefore, activating this plane is crucial to enable its commercial application. Doping strategies and defect engineering have proven capable of modulating local electronic states amplifying the HER activity. The present work addresses the direct synthesis of MoS_2 on the surface og carbon felt via impregnation and thermodecomposition and theoptimization of the material's electrocatalyticactivity for HER. Scanning electron microscopy characterization reveals the extensive distribution of MoS2 crystals on the carbon fiber surface and highlights the role of the carbon felt's 3D architecture, which provides a high specific surface area. The use of this material as a support is motivated by the pursuit of self-supported electrodes, where the electrical contact between the catalyst and the current collector is optimized, eliminating the need for external agents that may impact the system's conductivity. Raman spectroscopy analyses reveal the presence of structural defects associated to the MoS_2 2H phase. Preliminary linear sweep voltametry analyses demonstrate the synergistic effect between the support and the active phase, as well as the significant evolution of catalytic performance, even without prior felt activation.



SEM image of the modified carbon felt fibers

Agradecimentos/Acknowledgments

I acknowledge the SuperNano laboratory for all the research support and CAPES for the Master's program funding

PROPOSIÇÃO DE UM FLUIDO NÃO-NEWTONIANO COM COMPORTAMENTO SHEAR-THICKENING VISANDO APLICAÇÕES NA ÁREA DE POLIMENTO

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Palavras Chave:*Óxido de Cério(III), Polimento, Polietilenoglicol, Shear-Thickening.*

Highlights

Shear thickening fluids (STFs) are type of non-newtonian fluid characterized by an increase in viscosity under applied shear stress and when the shear stress is removed, it returns to a fluid state.

Resumo/Abstract

Fluidos não-newtonianos, especificamente, os que apresentam um comportamento denominado*shear-thickening,*são uma classe de materiais com propriedades específicas e com diversas aplicações, tais como: sistemas de proteção, proteção de impacto, controle de vibração, entre outras. O presente trabalho apresentará os desafios envolvidos no processo de fabricação de um fluido dilatante, ou seja, a fabricação de Shear Thickening Fluid (STF) com o propósito de obter um fluido para aplicações na área de polimento, por meio de um método conhecido como*Shear-Thickening Polishing (STP)*. O STP é um método recém estruturado e explora o comportamento dos fluidos dilatantes visando o tratamento de superfície de peças por meio de um polimento de alta-precisão. O método STP explora a transição de fluido para sólido, com a aplicação de esforços sobre o material e assim, promoverá a remoção de material da superfície da amostra, garantindo um controle de qualidade e reduzindo danos à superfície do objeto polido. O óxido de cério(III) foi utilizado como agente de polimento e foi obtido pelo método de coprecipitação. Duas vertentes foram utilizadas para o desenvolvimento de um fluido*shear-thickening*: (i) suspensão de amido e água, o qual é um fluido bem conhecido na literatura por apresentar este comportamento e (ii) um fluido de partículas de argila sódica dispersas em polietilenoglicol. A síntese pelo método de coprecipitação produziu partículas micrométricas de óxido de cério(III) com morfologias distintas (tubular e placa) e presença de aglomerados. Em relação as suspensões de amido, o comportamento*shear-thickening*foi observado de duas formas distintas: o chamado*shear-thickening*contínuo (CST) e*shear-thickening*descontínuo (DST). Já as suspensões de argila sódica não apresentaram um caráter dilatante e o comportamento reológico aproximou-se de um fluido com característica de um material pseudoplástico.

Agradecimentos/Acknowledgments

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PVP/VA electrospinning for fast release of nifedipine

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Palavras Chave:*Nanomaterials, Bioavailability, Electrospinning, Polymer, Drug,Nanomaterials,bioavailability,electrospininning,polymer,drug,Nanomaterials,Bioavailability,Electrospinning,Polymer,Drug*

Highlights

PVP/VA electrospun nanofibers loaded with NDP were successfully produced.

The 20% NDP formulation showed the best release profile.

The release kinetics followed the Fickian diffusion model.

Resumo/Abstract

Oral drug administration presents limitations for specific population groups, such as the elderly and children, who frequently manifest dysphagia or difficulty swallowing. In this context, fast-release dosage forms stand out by allowing the active ingredient to be absorbed directly into the systemic circulation. Such systems can be produced via the electrospinning technique, resulting in polymer matrices incorporated with the drug. The present study aimed to develop electrospun nanofibers composed of 35% (w/v) poly(1-vinylpyrrolidone-co-vinyl acetate) (PVP/VA), loaded with nifedipine (NDP) at ratios of 10%, 20%, and 30% (w/w). NDP is an antihypertensive drug with low water solubility. A mixture of ethanol and distilled water (97:3 v/v) was used as the solvent system. For the electrospinning process, the established operational parameters were: a flow rate of 1.5 mL h^{-1}, a voltage of 16 kV, and a distance of 12 cm between the needle and the metallic rotating collector. Morphological characterization via SEM revealed that the formulation presented more homogeneous fibers with a uniform diameter distribution. Thermal analyses (TGA and DSC) corroborated the thermal stability of the system and indicated the successful amorphous dispersion of NDP. FTIR spectra showed shifts in characteristic bands, suggesting the formation of hydrogen bonds and molecular interactions between the NDP and the polymer matrix.*In vitro*release studies in simulated saliva indicated that the kinetics followed the Fickian diffusion mechanism, with a satisfactory fit to the Weibull and Korsmeyer-Peppas models. The formulation with 20% NDP exhibited the most favorable release profile.

Agradecimentos/Acknowledgments

Acknowledgments to CAPES for the funding; to UNIOESTE, GIPeFEA, and GENPEC for the technical and institutional support.

Rational Design of Nickel-Glycerolates: Synthesis Optimization and Electrocatalytic Performance

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Palavras Chave:*Nickel glycerolates,Oxygen evolution reaction (OER),Synthesis optimization,Rational design,Structure-activity relationship*

Highlights

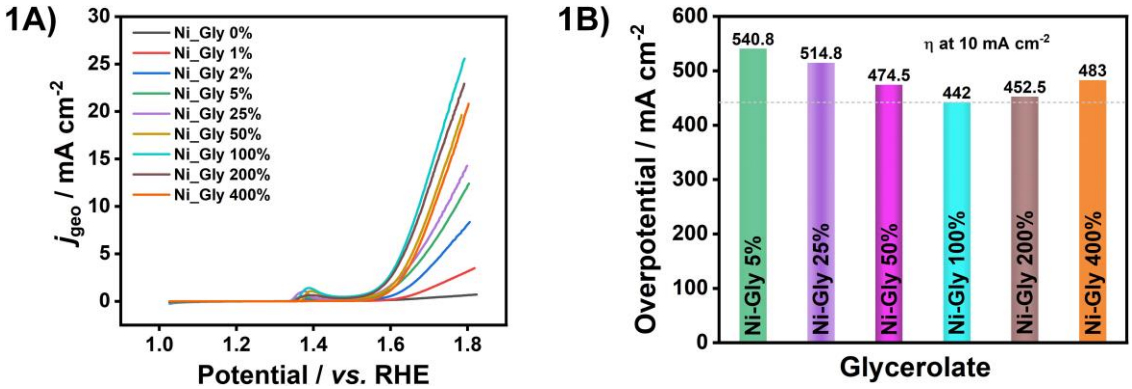
Rational Ni-glycerolates synthesis for OER catalysis.

Glycerol content tunes electrochemical performance.

Optimized Ni-Gly reached overpotential of 442 mV.

Resumo/Abstract

The design of electrode materials is a key strategy for improving the performance of energy conversion devices. In this context, coordination compounds (CCs), such as metal-glycerolates, stand out as highly versatile materials, enabling their direct use as electrode materials or as precursors for the synthesis of a broad range of functional materials with well-tailored morphologies, structures, and compositions. Although common, the solvothermal synthesis of metal-glycerolate-based materials often utilizes a large excess of glycerol. This work aimed to optimize glycerol use in the synthesis of nickel-glicerolate (Ni-Gly) and to evaluate the impact of this rational design on electrochemical performance in the oxygen evolution reaction (OER). The reference synthesis used 2.5 mmol of nickel nitrate and 8 mL of glycerol (which represents 100% glycerol) in an alcoholic medium. The resulting solution was subsequently loaded into a Teflon-lined stainless-steel autoclave and maintained at 180 °C for 6 h. Variations of 0%, 1%, 2%, 5%, 25%, 50%, 200%, and 400% of the initial glycerol concentration were also prepared. Interestingly, higher concentrations of glycerol stabilize smaller Ni-Glys, whereas in its absence, the size increases drastically. LSV curves (Figure 1A) and calculated overpotential (Figure 1B) demonstrate the superior performance of the Ni-Gly100% sample, which exhibited the lowest overpotential of 442 mV to reach 10 mA cm–². Although Ni-Gly100% exhibits the best electrochemical activity, higher glycerol content leads to lower-performing electrocatalysts with more agglomerated powders. Overall, this study demonstrates that a rational optimization of glycerol content is crucial for tailoring the electrochemical performance of Ni-Glys toward efficient OER catalysis. The results highlight Ni-Gly100% as an optimal balance between structural control and activity, while emphasizing that excessive glycerol is detrimental due to particle agglomeration.



1A - LSV curves/Figure 1B overpotential at a current density of 10 mA cm–2

Agradecimentos/Acknowledgments

This work was supported by the São Paulo Research Foundation (FAPESP processes 2023/17560-0, 2025/04952-3, 2025/15836-4, 2025/15526-5, 2023/00246-1).

Recent Advances in Spray-Drying Synthesis of Low-, Medium- and High-Entropy Layered Transition Metal Oxide Cathodes for Sodium-Ion Batteries

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Palavras Chave:*Spray-drying,Sodium-ion batteries,Cathode,Synthesis,High-Entropy Oxides*

Highlights

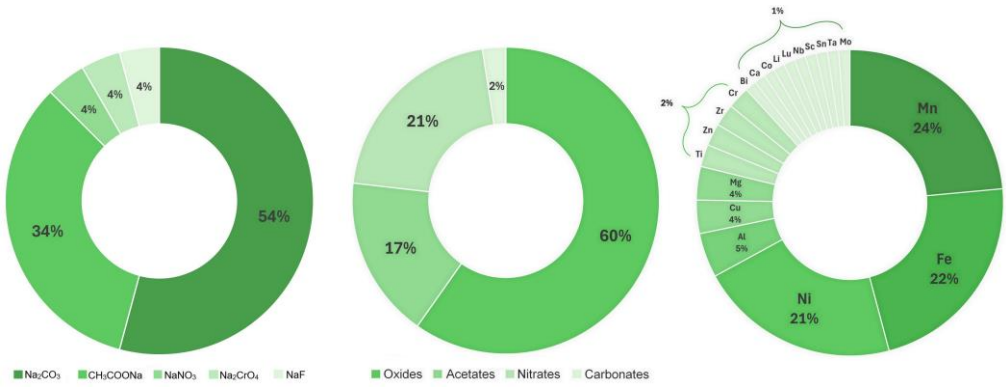
Review of spray-drying synthesis for entropy-designed Na_xTMO_2 cathodes.

Trends in precursors, processing and calcination are identified.

Improved reporting is needed for reproducibility and viability.

Resumo/Abstract

Sodium-ion batteries (SIBs) have emerged as promising alternatives to lithium-ion batteries due to the abundance of sodium, lower cost, and enhanced safety. To improve SIB performance, recent studies have explored entropy design in layered transition-metal oxides (Na_xTMO_2). In this context, spray-drying has been adopted to optimize synthesis, control morphology, and improve cathode efficiency. This work presents a literature-based analysis of studies published over the past five years on Na_xTMO_2 cathodes synthesized by spray-drying. The objective is to map synthesis strategies and identify trends in precursor selection, process parameters, thermal treatments, and chemical compositions. A systematic review of peer-reviewed articles was conducted, extracting data on precursors, spray-drying conditions, and calcination protocols, which were then comparatively analyzed. Na_2CO_3 is the main sodium source due to its versatility and industrial availability, accounting for nearly 54% of the reported compositions. On the other hand, metal oxides predominate as transition-metal precursors (around 60%) owing to higher thermal stability, lower cost, and absence of decomposition byproducts. Besides, Ni, Fe, and Mn are the most frequently used metals, combining structural stability, high capacity and voltage, abundance, and low toxicity. Spray-dryer inlet temperatures range from 150 to 290 °C and directly affect particle size. After spray-drying, precursors are typically subjected to one or two calcination steps between 400 and 980 °C to obtain the crystalline phase. Overall, this study highlights spray-drying as an efficient route for synthesizing entropy-designed Na_xTMO_2 cathodes. However, variability and insufficient reporting of synthesis parameters limit direct comparisons between studies. Standardization of conditions and optimization of synthesis and thermal steps are essential to improve reproducibility and industrial viability in this still largely unexplored field.



Sodium source, precursor, and metal distributions in spray-drying synthesis of NaxTMO2 to SIBs.

Agradecimentos/Acknowledgments

This work was supported by the São Paulo Research Foundation (FAPESP processes 2025/19781-0 and 2023/17560-0).

Reproducibility in Materials Synthesis: A Systematic Review and Meta-Analysis of AuNP Turkevich and MoS_2 CVD Methods

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Palavras Chave:*Reproducibility, Materials synthesis, Gold nanoparticles, MoS_2, Systematic review*

Highlights

Systematic review and meta-analysis reveal critical reproducibility gaps in AuNP Turkevich synthesis and MoS_2 CVD growth.

Resumo/Abstract

Reproducibility is a cornerstone of scientific research, yet it remains a persistent challenge in materials synthesis, particularly for nanomaterials whose properties are highly sensitive to experimental conditions. In this work, we present a systematic review and meta-analysis aimed at critically assessing the reproducibility of two widely used and often considered “standard” synthesis routes in materials science: the Turkevich method for gold nanoparticles (AuNPs) and the chemical vapor deposition (CVD) growth of molybdenum disulfide (MoS_2). An adapted PRISMA-based protocol combined with a modified SPIDER framework was employed to evaluate methodological transparency, parameter reporting, and outcome consistency across the literature. Comprehensive searches were conducted in Scopus and Web of Science databases, covering publications from 1999 onward. More than 1,300 articles related to AuNP synthesis and over 1,300 studies on MoS_2 CVD growth were initially retrieved and systematically screened using structured checklists and automated Python-based text classification tools validated against independent human reviewers. Our analysis reveals that, despite the extensive literature and the widespread perception of both methods as reproducible, only a limited fraction of studies rigorously address reproducibility at the synthesis level. Critical experimental parameters are frequently underreported, and statistical analyses of size, morphology, or thickness distributions are rarely included. These shortcomings significantly hinder inter-laboratory reproducibility and comparability. The results demonstrate the potential of systematic reviews and meta-analyses as powerful tools for diagnosing reproducibility challenges in materials synthesis and for guiding the development of more robust, transparent, and reproducible experimental protocols in nanomaterials research.

Agradecimentos/Acknowledgments

Alexander von Humboldt Foundation, CAPES, CNPq, FAPERJ, Serrapilheira Institute, and INCT/Nanocarbono are gratefully acknowledged.

Síntese, caracterização e emissão upconversion de nanopartículas de $Gd_2O_2S:Yb^{3+},Er^{3+}$ obtidas pelo método de decomposição térmica

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Palavras Chave:*lantanídeos, nanopartículas, upconversion*

Highlights

Síntese e caracterização fotofísica de nanopartículas de oxissulfetos de gadolínio dopado com os íons Yb^{3+} e Er^{3+} obtidas por meio do método de decomposição térmica, um estudo da emissão upconversion

Resumo/Abstract

Os oxissulfetos de gadolínio são excelentes matrizes para íons lantanídeos, sendo promissores em dispositivos optoeletrônicos devido à sua capacidade de emitir luz quando fotoexcitados. Quando dopados com os íons Yb^{3+} e Er^{3+} e submetidos à excitação no infravermelho próximo, exibem luminescência por conversão ascendente de energia (upconversion), processo no qual dois ou mais fótons de baixa energia são absorvidos, resultando na emissão de fótons de maior energia. A síntese dessas nanopartículas por decomposição térmica em solventes com altos pontos de ebulição (DTSAE) tem se mostrado altamente eficaz, permitindo controle sobre tamanho e forma, além de favorecer a formação de fases cristalinas puras sob condições brandas, diferentemente de métodos convencionais que exigem temperaturas superiores a 600 °C. Este estudo investiga a síntese e caracterização dessas nanopartículas, destacando a relevância DTSAE na obtenção de materiais com propriedades aprimoradas. Foram preparadas nanopartículas de oxissulfetos de Gd^{3+} dopado com Er^{3+} e Yb^{3+} e caracterizadas por FTIR, DRX e espectroscopia de fotoluminescência. A concentração de Yb^{3+} foi mantida em 20% e avaliou-se a influência da concentração de Er^{3+} (1, 2 e 4%) na emissão upconversion. As nanopartículas possuem fase cristalina hexagonal e após excitação em 980 nm, observaram-se as emissões no visível características do Er^{3+}. As curvas de decaimento de emissão exibiram comportamento biexponencial, com tempos de vida na faixa de 3 a 10 ns, valores típicos para esse tipo de sistema. O estudo da lei de potência confirmou que essas emissões seguem um processo upconversion. Entre as amostras avaliadas, as nanopartículas dopadas com 2% de Er^{3+} apresentaram a maior intensidade de emissão. Esses resultados reforçam que o método DTSAE é eficiente para controlar a fase cristalina e a dinâmica de transferência de energia no sistema $Gd_2O_2S:Yb^{3+}Er^{3+}$, permitindo otimizar suas propriedades luminescentes.

Agradecimentos/Acknowledgments

Os autores agradecem a CNPq (PIBIC), FAPESP, CAPES e LumiNanoTech.

Síntese e Caracterização de Nanopartículas de Óxido de Ferro para Extração de Ácido Desoxirribonucleico

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Palavras Chave:*Nanopartículas, óxido de ferro, magnetita, extração, DNA,Nanopartículas, óxido de ferro, magnetita, extração, DNA*

Highlights

Síntese e caracterização de nanopartículas de magnetita. Aplicação eficiente de nanopartículas na extração em fase sólida de DNA. Eficiência de extração comprovada por PCR em tempo real.

Resumo/Abstract

O desenvolvimento de novas metodologias para a extração do DNA com maior pureza e integridade vem se tornando cada vez mais necessário, visto a importância do conhecimento estrutural da biomolécula para o estudo das diversas doenças genéticas já reportadas na literatura. O uso de reagentes tóxicos, solventes em grandes quantidades e procedimentos laboratoriais exaustivos são os principais desafios que as novas metodologias buscam superar. Por isso, o uso de nanopartículas de óxido de ferro (MNPs), especialmente as magnéticas, tem sido proposto como alternativa para promover a extração do DNA de forma rápida e eficiente. Neste trabalho, as MNPs foram sintetizadas pelo método de coprecipitação e caracterizadas por microscopias eletrônicas de varredura e transmissão (SEM e TEM), difração de raios X (XRD) e espectroscopia no infravermelho (FTIR). As MNPs foram aplicadas na extração em fase sólida do DNA, com eficiência estudada por PCR em tempo real. Conforme observado nas imagens de SEM e TEM, o diâmetro das MNPs variou entre 10 e 30 nm. A fase cristalina magnetita foi confirmada por XRD e FTIR, a partir do padrão cristalográfico e das bandas características do óxido de ferro. As MNPs foram capazes de isolar o material genético da porção aquosa da amostra de DNA, sendo que o tempo de dessorção de 10 min resultou em maior eficiência de extração. O aumento do volume de extração não melhorou a captura do DNA, contribuindo para o desenvolvimento de sistemas miniaturizados, com menor uso de materiais tóxicos e geração de resíduos químicos. Os resultados confirmam a capacidade das MNPs de extrair o DNA com eficiência de amostras aquosas e evidenciam o potencial da nanociência no desenvolvimento de materiais sustentáveis, além de aumentar as perspectivas de otimização dos parâmetros experimentais por meio da funcionalização das MNPs, visando a estabilidade coloidal e um sistema de extração de alto desempenho.

Agradecimentos/Acknowledgments

Os autores agradecem à UFCSPA pela infraestrutura e a FAPERGS e CNPq pelo apoio financeiro para a execução desta pesquisa.

Síntese e luminescência de novos derivados do 1,3,4-oxadiazol

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Palavras Chave:*heterocíclico aromático, síntese orgânica, mesógeno, propriedades fotofísicas*

Highlights

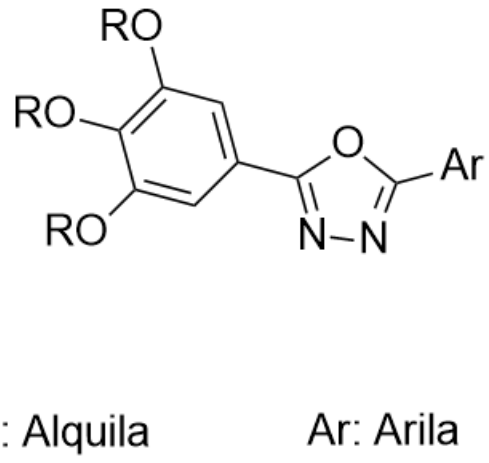
Synthesis of new 1,3,4-oxadiazole derivatives for studying photophysical and mesogenic properties

Intermediate products currently being characterized

Three different synthetic routes being investigated

Resumo/Abstract

Oxadiazóis são heterociclos aromáticos com fórmula molecular básica $C_2H_2N_2O$. Esses compostos têm demonstrado importância prática em diferentes áreas, como química medicinal, com derivados que apresentam propriedades antitumoral, e química de materiais, com derivados que apresentam características líquido-cristalinas e luminescência. Nosso grupo tem preparado derivados 1,3,4-oxadiazólicos com propriedades luminescentes, líquido-cristalinas e ópticas não-lineares com a característica de possuírem uma porção aromática e anexado a essa um grupo éter alifático. Este trabalho visa sintetizar e caracterizar 1,3,4-oxadiazóis com diferentes grupos aromáticos na posição 2 (2-, 3- e 4- piridinil) e estudar suas propriedades fotofísicas. Em comparação aos derivados já sintetizados, os novos compostos possuem em sua estrutura três grupamentos éter de cadeia longa, que poderiam auxiliar na criação da mesofase. Além disso, esses grupos são ativadores do anel aromático e, portanto, é esperado que haja um deslocamento nos espectros de emissão em relação aos derivados já descritos. Diferentes abordagens sintéticas foram exploradas na tentativa determinar a mais eficiente e com isso foi possível definir a rota utilizada nesse trabalho. As primeiras três etapas foram realizadas com êxito, levando aos compostos desejados em bons rendimentos. Todos os compostos sintetizados foram caracterizados através de RMN e FTIR. Análises térmicas e de luminescência serão realizadas futuramente.



Representação do derivado do 1,3,4-oxadiazol alvo desse trabalho

Agradecimentos/Acknowledgments

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Singlet Oxygen Generation under X-ray Irradiation from a Ru(II)-Functionalized Radioluminescent Lanthanum MOF for Photodynamic Therapy

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Palavras Chave:*Metal–organic frameworks,singlet oxygen,photosensitizer,X-ray–activated photodynamic therapy,cancer therapy*

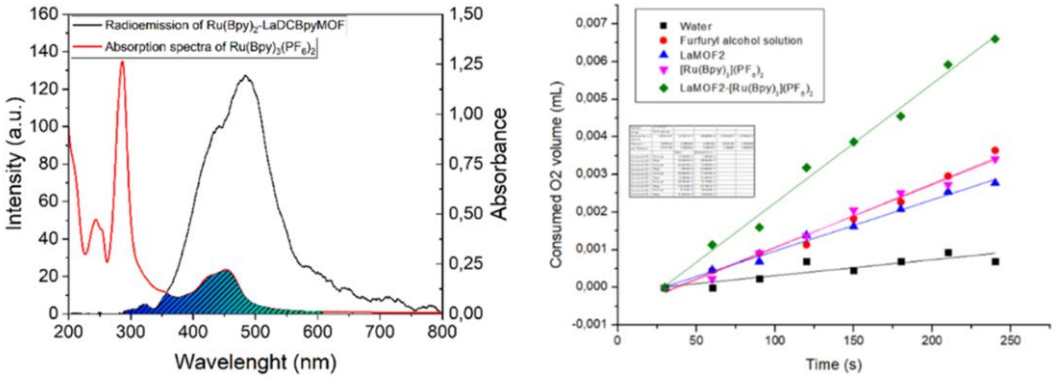
Highlights

X-PDT is enabled by a radioluminescent La-based MOF integrating a Ru(II) photosensitizer; Efficient ROS generation achieved via intraparticle energy transfer under X-ray irradiation.

Resumo/Abstract

Photodynamic therapy relies on the localized activation of photosensitizers (PS) to generate reactive oxygen species (ROS); however, its clinical applicability is constrained by the limited penetration depth of optical radiation in deep tissues. X-ray activated photodynamic therapy (X-PDT) has therefore emerged as a promising alternative, as ionizing radiation can effectively penetrate all human tissues. In this context, the development of photosensitizers that can be efficiently activated by ionizing radiation represents a critical requirement for the advancement of X-PDT. Perhaps, the key of this process involves energy transfer process. An innovative strategy to address this challenge involves the use of radioluminescent metal-organic framework (RL-MOF) platforms capable of transferring energy to well-established PS. Herein, we report the synthesis of $Ru(Bpy)_2$–LaMOF, a lanthanum-based RL-MOF incorporating a ruthenium PS complex, which combines structural robustness, efficient intraparticle energy transfer, and enhanced ROS generation under ionizing radiation. The material was comprehensively characterized by infrared spectroscopy, powder X-ray diffraction, differential pulse voltammetry, dynamic light scattering, scanning and transmission electron microscopy (SEM/TEM), and elemental analysis by SEM-EDS and ICP-OES. Structural and morphological analyses confirmed that incorporation of the Ru complex occurred without disruption of the MOF framework. ROS generation was evaluated by monitoring oxygen consumption using a selective singlet oxygen scavenger under light and X-ray irradiation. While LaMOF did not show oxygen consumption, $Ru(Bpy)_2$–LaMOF showed pronounced O_2 depletion, under light and ionizing radiation, consistent with efficient intraparticle energy transfer. Cell viability assays revealed that light irradiation induced higher cytotoxicity, highlighting the need for further optimization of PDT parameters.

Reference: Dhaini, B. et al.**Pharmaceuticals**, 2025.



Energy transfer in $Ru(Bpy)_2$–LaDCBpyMOF and O_2 consumption under X-rays for MOFs and controls.

Agradecimentos/Acknowledgments

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SnO2 for detection of volatile organic compounds from food degradation.

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Palavras Chave:*Gas sensors, tin (IV) dioxide, MVOCs, acetone, food degradation.*

Highlights

Synthesis of SnO_2 by microwave-assisted hydrothermal method.
Significant response for the detection of acetone at 1 ppm.
Detection of volatile organic compounds associated with food degradation.

Resumo/Abstract

This study aims to synthesize and investigate tin (IV) oxide as a sensor for detecting microbial volatile organic compounds (MVOCs) released during the degradation of foods such as fruits and meats. Among these MVOCs, triethylamine (TEA) stands out as a compound commonly associated with the spoilage of seafood, characterized by a pungent odor of rotten fish and linked to adverse effects on human health, such as gastroenteritis and headaches. For the detection of these compounds, SnO_2 is widely used as a sensor due to its low cost and ease of operation. To this end, we synthesized SnO_2 by a microwave-assisted hydrothermal method, using urea and polyvinylpyrrolidone (PVP) K-30 for morphological control and nanoparticle growth. The precipitate obtained was heated to 400 °C for thermal decomposition. FTIR and SEM analyses were performed to characterize the sample's composition and morphology. Preliminary results confirm the formation of the tetragonal crystalline phase of SnO_2 after calcination at 400 °C, in contrast to the precursor material, which showed a mixture of phases. The performance of the precursor and SnO_2 as sensors was evaluated by exposure to 1 ppm of 3-methyl-1-butanol, triethylamine, acetone, isoprene, ethanol, benzene, toluene, and*m*-xylene at operating temperatures of 250-400 °C. A response of 36.17 was observed for acetone gas at 1 ppm at an operating temperature of 300 °C. Therefore, the precursor demonstrates good performance as a sensor for MVOCs.

Agradecimentos/Acknowledgments

This research was supported by CNPq (149558/2025-2), CNPq (Process 305542-2024-9), and FAPESP (2020-06421-1).

Sodium alginate biofilms cross-linked with Fe^{3+}: effect of Iron(III) concentration.

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Palavras Chave:*Sodium alginate, Biofilms, Ionic crosslinking, Iron (III), Stability*

Highlights

Sodium alginate biofilms were ionically crosslinked with Fe^{3+}.

Crosslinking promoted water and thermal stability.

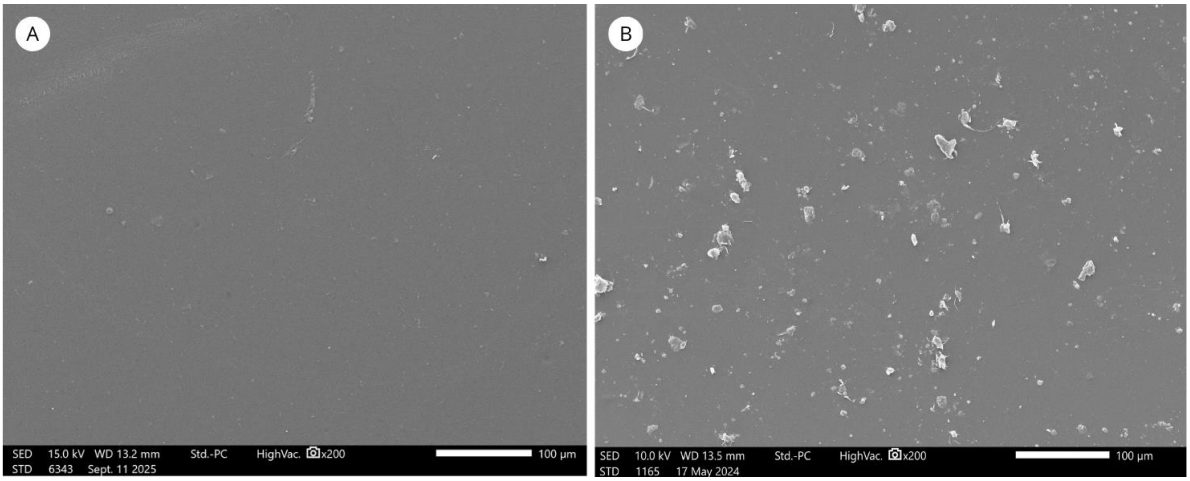
Structural reorganization was evidenced by FTIR and SEM analyses.

Resumo/Abstract

Sodium alginate (SA) is a hydrophilic biopolymer extracted from brown algae, widely used due to its gelation, viscosity and water retention properties. Ionic crosslinking improves properties such as mechanical strength and stability in aqueous environments. Among the ions employed in the crosslinking process, iron(III) (Fe^{3+}) enables the incorporation of functional properties into the polymer matrix, allowing applications in environmental areas, such as pollutant adsorption.

This work aimed to develop and characterize $FeCl_3$-crosslinked SA biofilms by evaluating the concentration of the crosslinking agent. Swelling index measurements, TGA, SEM and FTIR analyses were used. The biofilms were prepared from a 2% (w/v) aqueous SA solution, dried, and subsequently immersed in $FeCl_3$ solutions at 2% and 5% for 20 minutes to promote crosslinking.

The swelling index indicated stable behavior of the crosslinked biofilms in aqueous media, with low water uptake. Thermogravimetric analysis showed thermal stability up to approximately 200 °C. SEM images revealed a dense structure, with higher surface homogeneity for the biofilm crosslinked with 2%, whereas the 5% sample exhibited a higher presence of particulate domains. FTIR spectroscopy showed changes in the characteristic alginate bands, with shifts in position and intensity after crosslinking, indicating ionic interactions between Fe^{3+} and the polymer matrix and reorganization of the polymer network. Considering process efficiency, ease of control and cost reduction, the 2% concentration was found to be suitable for future steps. Overall, the results demonstrate that Fe^{3+} crosslinking was effective, yielding a material with potential application in pollutant adsorption processes.



SEM images of SA biofilms crosslinked with $FeCl_3$ at 2% (A) and 5% (B). Magnification: 200×.

Agradecimentos/Acknowledgments

The authors acknowledge CNPq, FAPESC, UDESC, and the Laboratory of Materials Development (LDM).

Solvothermal Synthesis of a Yttrium-Based Metal–Organic Framework via In Situ Linker Formation

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Palavras Chave: *Yttrium-based MOF, In situ synthesis, Solvothermal synthesis,,Yttrium-based MOF,In situ synthesis,Solvothermal synthesis*

Highlights

Crystalline yttrium-based MOF obtained via *in situ* linker formation. Framework contraction yields smaller pores than Zr analogues. Microporous materials with BET areas up to 880 $m^2 \cdot g^{-1}$ were achieved.

Resumo/Abstract

A yttrium-based metal–organic framework (MOF) was synthesized via solvothermal methods using an *in situ* organic linker formation approach from simple aromatic precursors. The study focused exclusively on yttrium nitrate as the metal source, while the influence of modulators, co-modulators, solvent choice, and controlled water addition was systematically investigated to promote crystallization and porosity.

Powder X-ray diffraction confirmed the formation of a crystalline MOF under optimized conditions, exhibiting characteristic low-angle reflections typical of porous frameworks. A systematic shift of diffraction peaks toward higher 2θ values, relative to a known zirconium-based analogue, indicates significant unit cell contraction arising from the substitution of Zr(IV) by Y(III), resulting in shorter interplanar distances and smaller crystallite sizes. Optical microscopy revealed microcrystalline powders with predominantly octahedral morphology.

Nitrogen adsorption–desorption measurements at 77 K demonstrated permanent microporosity with Type I isotherms and BET surface areas of up to 880 $m^2 \cdot g^{-1}$ after optimization. Pore size distribution analysis revealed contracted micropores, consistent with framework contraction and partial pore obstruction by capping species or trapped solvent-derived cations. Water was identified as a critical modulator, with small, controlled amounts enhancing crystallinity, while excess water led to amorphous, nonporous impurities.

This work establishes synthetic conditions for a new yttrium-based MOF obtained via in situ linker formation. The study is ongoing, and future investigations will address its application in photopolymerization systems and 3D printing.

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Spray-Dried Vinasse as a Sustainable Feedstock for Organomineral Fertilizer Development

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Palavras Chave:*Powder vinasse, sugarcane bagasse ash, atomization, agro nutrients.,Powder vinasse,,sugarcane bagasse ash,,atomization,,agro nutrients.*

Highlights

Vinasse microparticles treated by sugarcane bagasse ash with potential for use as organomineral fertilizer.

Conversion of vinasse into solid microparticles via spray drying.

Resumo/Abstract

The sugar-energy industry generates substantial byproducts, notably vinasse and sugarcane bagasse ash (SCBA). While vinasse is commonly used for fertigation due to its nutrients, its high pollution potential necessitates strict regulation. This study investigated the addition of 5% (w/v) SCBA to vinasse, followed by 48 h of shaker, centrifugation, filtration, and spray drying to produce solid vinasse microparticles. The resulting microparticles and ash were characterized using TG-DTG, FTIR, XRD, SEM, and organomineral analyses. Results showed compositional changes indicating nutrient exchange between vinasse and ash. The final microparticles contained 9% potassium, 28% organic matter, nitrogen, phosphorus, and micronutrients, highlighting their potential as organomineral fertilizers. Ash stabilization and spray drying reduced vinasse's liquid fraction by 93%, concentrating it into about 7% solids and improving its stability, transportability, and fertilizing potential.

Agradecimentos/Acknowledgments

The authors are grateful to the São Paulo Research Foundation, FAPESP-Brazil (Process Number 2024/080369) for financial support.

STRUCTURAL TRANSFORMATIONS IN RENEWABLE FOAMS DURING BIODEGRADATION EVALUATED BY FTIR

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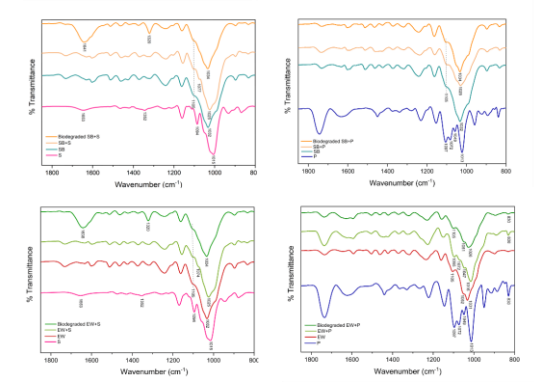
Palavras Chave:*FTIR (Fourier Transform Infrared Spectroscopy),Foams,Biopolymers,Biodegradation,Lignocellulosic residues*

Highlights

Starch-and pectin-based foams exhibit performance comparable to conventional plastic foams, while offering environmental Sustainability and end-of-life biodegradability.

Resumo/Abstract

Synthetic foams derived from petrochemicals are widely used in packaging and disposable products but pose significant environmental impacts due to their extremely slow biodegradation. As an alternative, renewable foams produced from lignocellulosic residues, such as sugarcane bagasse (SB) and eucalyptus wastes (EW), offer a more sustainable solution. In this study, foams were prepared using different components, combining unrefined SB and EW particles with biopolymers, starch, and pectin. The foams' biodegradability was tested in soil using Bartha's respirometers, which measured CO_2 production as evidence of biodegradation. The foams biodegraded efficiently, with kinetics depending on composition. Kinetic analysis using the Gompertz model revealed shorter lag times for SB-based foams (0.09–5.8 days) compared to EW-based foams (12.4–19.5 days). Fourier Transform Infrared Spectroscopy (FTIR) was used to assess the chemical environment of foams before and after biodegradation in soil. The results showed that in starch-based foams, significant modifications occurred in bands associated with water absorption, suggesting increased interactions with water after cleavage of glycosidic bonds. This exposed new hydroxyl groups and increased the material's porosity and water retention. There was also evidence of material loss and significant structural rearrangements, indicating deep transformations in starch. In contrast, pectin-based foams showed only minor structural modifications, suggesting a slower degradation process and better maintenance of the material's integrity. Pectin biodegraded more slowly and less intensely than starch due to its highly branched, heterogeneous structure, which hindered enzymatic access. This study provides insights into developing foams with tailored biodegradation for packaging applications, balancing in-use performance and post-disposal biodegradation to suit the product's shelf life.



FTIR spectra of starch- or pectin-based foams with SB or EW before and after biodegradation.

Agradecimentos/Acknowledgments

FAPESP through the Young Investigators Grant (23/09659-7), and the Research, Innovation and Dissemination Center for Molecular Engineering for Advanced Materials – CEMol (Grant CEPID No. 2024/00989-7). VBPS thanks the scholarship FAPESP 23/14118-5.

Study of The Optical Properties of 2D Hybrid Nanomaterials Based on Few-Layer Graphene and Graphitic Carbon Nitride (g-C_3N_4) and its Derivatives

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Palavras Chave:*Optical Properties,g-C_3N_4,graphene,2D Hybrid Nanomaterials*

Highlights

-g-C_3N_4/graphene hybrids show tunable band gap and modulated PL.

-Interfacial coupling reduces defects or promotes charge transfer.

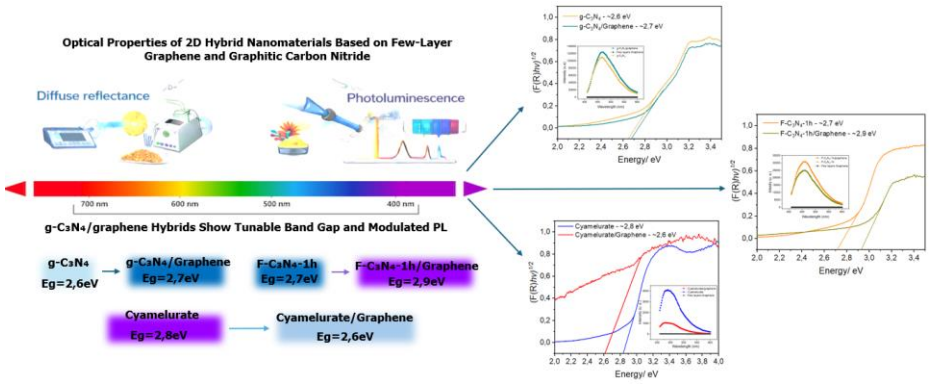
-Potential for photocatalysis and optoelectronic devices.

Resumo/Abstract

Hybrid materials based on 2D systems, such as few-layer graphene and g-C_3N_4 and its derivatives (fragmented g-C_3N_4 (F-C_3N_4-1h) and cyamelurate), have attracted significant scientific interest due to their complementary physicochemical properties[1],[2]. Despite their potential, the development of these systems still requires a deeper understanding of interfacial interactions and electronic coupling between their constituents. This work evaluated the optical properties of these hybrids by diffuse reflectance spectroscopy (Kubelka–Munk and Tauc) and photoluminescence spectroscopy. g-C_3N_4 exhibited an Eg of approximately 2.6 eV and a broad emission in the visible region (~470 nm), associated with π–π* transitions of heptazine units. In the g-C_3N_4/graphene, the shift of Eg to about 2.7 eV and the sharper optical absorption edge indicate a reduction in sub-gap states and defects, reflected in the increased PL intensity. The F-C_3N_4-1h derivative also showed an Eg around 2.7 eV and intense visible emission, resulting from structural fragmentation and modifications in the density of electronic states. In contrast, the F-C_3N_4-1h/graphene exhibited an increase in Eg to approximately 2.9 eV, while PL was suppressed, evidencing interfacial charge transfer and improved carrier separation. Cyamelurate presented an Eg close to 2.8 eV and intense visible emission typical of conjugated systems with localized electronic states. In the cyamelurate/graphene a reduction of Eg to about 2.6 eV and strong PL suppression were observed, indicating the formation of interfacial states and the role of graphene as an electron acceptor. Overall, the results demonstrate that hybridization modulates the electronic structure, either reducing defects and enhancing emission or promoting charge transfer and carrier separation, highlighting the potential of these systems for applications in photocatalysis and optoelectronic devices.

[1]Carbon, 214(2023), 118366,

[2]Applied Surface Science, 606 (2022), 154938.



Illustrative scheme of the study of the optical properties of 2D hybrid nanomaterials.

Agradecimentos/Acknowledgments

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Surface Enhanced Raman Spectroscopy of Gold nanoparticles deposited on High Entropy 2D Transition Metal Dichalcogenide

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Palavras Chave:*Gold nanoparticles,SERS,TMDs,Sensor*

Highlights

TMDs arise as new substracts for nanomaterial homogeneous deposition. Well distributed AuNP is key to Raman enhancement (SERS). Interaction between AuNP and TMDs might further increase Raman signal.

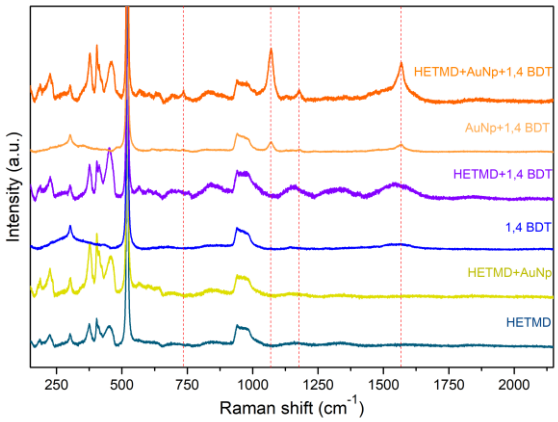
Resumo/Abstract

Nanopartículas de ouro (AuNPs) com diferentes morfologias despertam grande interesse em sensores ópticos devido às suas propriedades plasmônicas, que possibilitam a intensificação do espalhamento Raman e a detecção de analitos em baixas concentrações. O desempenho de substratos SERS está diretamente associado à formação de*hot spots*, dependente da densidade, morfologia e espaçamento entre as nanopartículas. Entretanto, a deposição homogênea e reprodutível de AuNPs ainda é um desafio para a produção em larga escala, sobretudo devido à baixa reprodutibilidade e ao alto custo de técnicas sofisticadas.

Nesse contexto, dicalcogenetos de metais de transição (TMDs), especialmente os sulfurados, destacam-se como substratos promissores, uma vez que a forte interação entre ouro e enxofre favorece a deposição homogênea de AuNPs, resultando em elevada concentração de*hot spots*. Além disso, a coordenação das AuNPs na superfície dos TMDs pode promover maior intensificação do sinal SERS por meio do mecanismo de transferência de carga.

Este trabalho tem como objetivo estabelecer um protocolo simples e reprodutível para a deposição de AuNPs sobre substratos de silício contendo cristais de MoS_2 pristino e de alta entropia dopados com V, W, Nb e Ta (HETMD), sintetizados por deposição química a vapor. A intensificação do sinal Raman foi avaliada utilizando 1,4-benzenoditiol (BDT) como molécula modelo, comparando os fatores de intensificação de substratos AuNP, MoS_2@AuNP e HETMD@AuNP.

Resultados preliminares de AFM e espectroscopia Raman (λ = 633 nm) indicam alta densidade de deposição de AuNPs com baixa agregação, bem como elevada intensificação dos modos vibracionais do BDT. Observa-se ainda aumento adicional do sinal em regiões de interação entre TMD e AuNPs, sugerindo contribuição do mecanismo químico via transferência de carga TMD–AuNP, atuando de forma sinérgica ao mecanismo eletromagnético na intensificação SERS.



Intensificação Raman 633 nm de BDT em MoS2 dopado com metais de transição e AuNPs.

Agradecimentos/Acknowledgments

CNPq, Serrapilheira, IQ-UFRJ.

Suspension-stable crystalline carbon nitride applied in photocatalytic reactions

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Palavras Chave:*Carbon Nitride,Photocatalysis,Single-Atom,Hydrogenation,Quasi-Homogeneous*

Highlights

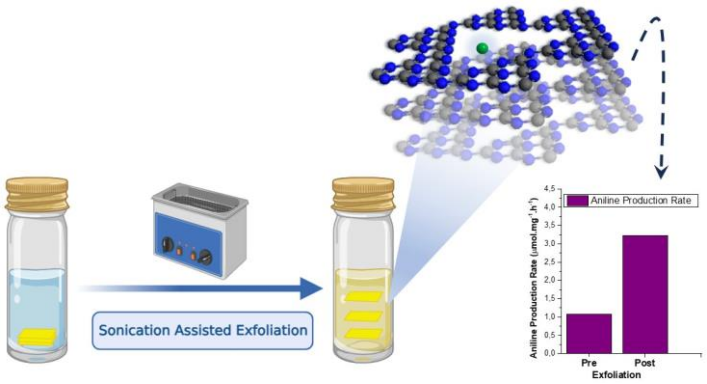
Photocatalytic activity improvement by the mechanical exfoliation of crystalline carbon nitride, yielding quasi-homogeneous systems

200% enhancement in photocatalyst activity post exfoliation

Resumo/Abstract

Catalysis, a key component in over 90% industrial processes, plays a fundamental role in the progress of science by enabling once unachievable chemical transformations. Photocatalysis is an elegant approach, providing a pathway for solar-to-chemical energy conversion through photo-harvesting materials such as crystalline carbon nitrides, which act as supports for single-atom photocatalysis when in poly(heptazine imide) (PHI) form. As a heterogeneous photocatalyst, PHI displays advantages including high thermal stability, recyclability, and outstanding semiconductor properties. However, a catalyst's performance is strongly influenced by the relationship between its physical state and the reaction medium, dictating diffusion, active sites accessibility, and charge transfer efficiency. In conventional heterogeneous systems, charge recombination and low dispersibility can limit the efficient use of photoexcited electrons and active sites. These drawbacks can be mitigated by engineering quasi-homogeneous systems.

Highly dispersive PHI was obtained by adding potassium chloride during synthesis, yielding Na/K-PHI, as opposed to the conventional melamine and NaCl thermal treatment that produces Na-PHI. Potassium ions increase the interlayer distance between PHI sheets and induce cyanamide defects, causing superficial charges that enhance water diffusion. Cation exchange of Na+/K+ by Ni^{2+} or Fe^{3+} provided Ni-PHI and Fe-PHI, which were exfoliated by ultrasonic treatment for 12h. X-Ray Powder Diffraction (XRD) revealed a more organized 3D stacking for Na/K-PHI, compared to Na-PHI. FTIR confirmed an increase in cyanimide groups in Na/K-PHI. Exfoliated Ni-PHI and Fe-PHI showed no decantation after two weeks, indicating high colloidal stability. Exfoliated Ni-PHI was tested in nitrobenzene reduction using water as proton source and glycerol as electron donor, exfoliation increased the aniline production rate from 1.08 to 3.23 $\mu mol \cdot mg^{-1} \cdot h^{-1}$.



Schematic representation of the developed work

Agradecimentos/Acknowledgments

We thank FAPESP, CNPq, CAPES and FINEP for financial support, and LabIvo, UFSCar, and the Department of Chemistry for providing infrastructure and research facilities.

Sustainable Biodegradable Foams from HPMC and Malt Fiber: A Green Alternative for Eco-Friendly Food Packaging

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Palavras Chave:*Packaging, polymers, cellulose, malt, agro-industrial residue,Packaging,cellulose,, malt,agro-industrial residue*

Highlights

Biodegradable packaging developed from HPMC and malt fiber. Incorporation of agroindustrial residue for mechanical reinforcement and barrier properties. Non-toxic biodegradation to soil.

Resumo/Abstract

Packaging based on petroleum-derived polymers is widely used by industry due to its high mechanical strength and good barrier properties; however, improper disposal and long degradation times lead to negative impacts on the environment and human health [1]. In this context, this study evaluated the development of biodegradable packaging based on natural polymers, specifically hydroxypropyl methylcellulose (HPMC) combined with agroindustrial malt fiber residue. Formulations were prepared with 8% ($m \cdot v^{-1}$) HPMC and 1 and 3% ($m \cdot v^{-1}$) malt fiber after prior fiber treatment, following the methodology described by Beninia et al. [2], resulting in homogeneous and aerated foams subsequently subjected to thermal treatment to promote thermoexpansion. The potential release of toxic byproducts was assessed through a germination test using common bean seeds (*Phaseolus vulgaris*), employing soil from the biodegradation assay as substrate, in accordance with the Rules for Seed Analysis (RAS, 2025) [3]. Germination rates ranged from 88.50% to 86.50% for fiber-containing materials, with no statistically significant difference compared to the control (84.50%), indicating the absence of toxicity [4]. These results, combined with color changes and other analyses performed by the authors, demonstrate the potential of malt fiber as a reinforcing agent in biodegradable packaging, contributing to the valorization of agroindustrial residues and the reduction of environmental impacts associated with petroleum-based packaging.

[1].*DOI: 10.1002/cl2.1033.*
[2]. DOI: 10.1016/j.proeng.2011.04.536.
[3]. DOI: 10.1016/j.cpb.2025.100557.
[4]. DOI: 10.1016/j.eja.2007.09.003.

Agradecimentos/Acknowledgments

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Sustainable preparation of PCL building blocks for the synthesis of PCL-PLA copolymers

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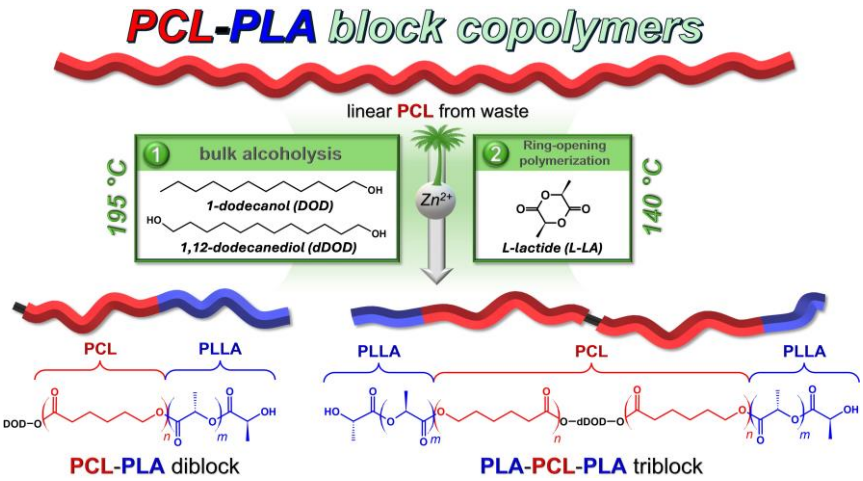
Palavras Chave:*Functional upcycling,Transesterification,Polyesters,Poly(caprolactone),Poly(lactic acid)*

Highlights

PCL bulk alcoholysis using fatty alcohols enables the production of tailored oligomers. The PCL oligomers are used to produce PCL-PLA block copolymers with different structures.

Resumo/Abstract

Despite its many advantages over other bioplastics, poly(ε-caprolactone) (PCL) still faces limited applications and a lack of sustainable chemical recycling routes that could extend its life cycle, reduce its carbon footprint, and enhance its applicability. To address this gap, a novel bulk alcoholysis process was developed for upcycling PCL into functional hydroxyl-terminated oligomers using two bio-based fatty alcohols, 1-dodecanol and 1,12-dodecandiol, in the presence of zinc stearate as a catalyst. This approach enables precise control over the final properties of the resulting oligomers by varying the type and the concentration of the alcohol, yielding mono- and difunctional telechelic structures suitable for further synthesis. The prepared PCL-based oligomers were used directly, without purification, as macroinitiators for the ring-opening polymerization (ROP) of L-lactide to synthesize well-defined diblock (PCL-PLA) and triblock (PLA-PCL-PLA) copolymers with a PCL/PLA ratio of 1 and tailored chain lengths. These copolymers were then applied in two different scenarios. The diblock copolymers were tested as compatibilizers for PLA/PCL blends, where they enhanced the elongation at break by improving interfacial adhesion between the two polymer phases. Moreover, two telechelic systems, namely a PCL oligomer and a PLA-PCL-PLA copolymer, were used in the preparation of thermoplastic polyurethanes (TPUs) via chain-extension reactions with methylene diphenyl diisocyanate (MDI), leveraging the residual catalyst and demonstrating efficient polymerization. Overall, the developed approach provides a robust, solvent-free, scalable, and effective strategy for valorising PCL waste, establishing a platform for producing sustainable, functional polyester-based building blocks.



Scheme of the functional upcycling of PCL to prepare PCL-PLA block copolymers

Agradecimentos/Acknowledgments

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Sustainable synthesis of controlled-release glass fertilizers using recycled glass as a silica source

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Palavras Chave:*Glass fertilizers,Controlled release,Recyclable glass,Sustainability,Nutrient release kinetics*

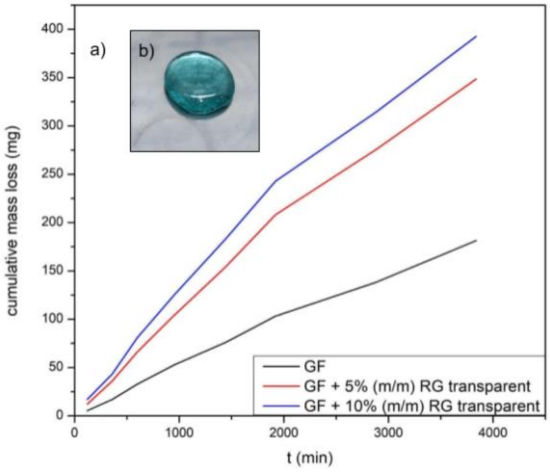
Highlights

Phosphosilicate glasses enable the tailored, controlled release of essential nutrients.

Post-consumer transparent glass is successfully repurposed as an eco-friendly silicon source.

Resumo/Abstract

Glass fertilizers (GFs) have emerged as a strategic technology to minimize nutrient leaching caused by the high solubility of conventional fertilizers, addressing the global demand for sustainable food production [1]. While GFs offer a versatile platform for adjusting release rates to plant needs [2-3], their scalability still depends on high-purity chemical reagents that increase the final production cost. In this sense, this work investigates the production of GFs incorporating macro and micronutrients into a matrix using recyclable transparent glass (RG) as the primary silicon (Si) source. SiO2 acts as a crucial network former and provides plants with physical resistance and improved phosphorus absorption. Utilizing waste glass addresses the environmental challenge in Brazil, where only a small fraction of commercial glass is recycled [4]. The glasses were synthesized via the melt-quenching method with Si (from RG) incorporated at 5% and 10% proportions. The resulting materials were ground and sieved (0.5–1.0 mm). Release tests were conducted using 100 mg of glass in 10 mL of solvent (ultrapure water and citric acid/sodium citrate buffer) under constant agitation (100 rpm) for 2 to 64 h. Multi-elemental quantification was performed via ICP-OES, while the remaining solid fractions were dried at 100 °C and subjected to chemical and morphological characterization. Preliminary results indicate that dissolution is controlled by cumulative mass loss and is significantly influenced by Si content. Increased silica modulation altered the glass network connectivity, directly impacting the physicochemical properties, release kinetics, and surface morphology of the fertilizers.



Cumulative mass loss as function of exposure time in the buffer solution of the vitreous fertilizer

Agradecimentos/Acknowledgments

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Sustainable Synthesis of Fluorescent Bioalginate from Amazonian Residues for Mercury Adsorption and Detection

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Palavras Chave:*Fluorescent Bioalginate,Amazonian Residues,Metallic Contaminants,Water Remediation,Adsorption*

Highlights

Sustainable synthesis of fluorescent bioalginate using agro-residues
High efficiency in removing potentially toxic metals from complex aqueous matrices
Fluorescent properties for monitoring processes

Resumo/Abstract

Water contamination by mercury (Hg^{2+}) in the Amazon region, driven by illegal mining and industrial activities, requires remediation solutions that are both environmentally friendly and economically viable. This work reports the development of a bifunctional nanocomposite (adsorbent and sensor) consisting of bacterial bioalginate and Carbon Quantum Dots (C-dots). The biopolymer was obtained via submerged fermentation by*Pseudomonas stutzeri*, using residual andiroba cake (*Carapa guianensis*) as a low-cost alternative substrate, resulting in a production yield of 4.8 g L^{-1}. Subsequently, the matrix was doped*in situ*with nitrogen-functionalized C-dots to confer fluorescent properties. Morphological characterization by SEM revealed that the pure bioalginate had a smooth, laminar surface, while the BioAlg@C-dots composite exhibited a rough and textured topography, indicating successful surface modification. TEM analysis confirmed the homogeneous dispersion of spherical C-dot nanoparticles (average diameter 4.2 ± 0.5 nm) anchored in the polymer network. BET porosimetry demonstrated a substantial increase in specific surface area, from 12.4 m^2 g^{-1} in the pure biopolymer to 48.7 m^2 g^{-1} in the nanocomposite, with predominant formation of mesopores (8.5 nm), facilitating intraparticle diffusion.
In remediation tests, the composite demonstrated high affinity for Hg^{2+}. Adsorption kinetics were rapid, reaching equilibrium in 45 minutes, fitting the pseudo-second-order model (R^2 > 0.999), suggesting chemisorption via complexation. Isotherms followed the Langmuir model, reaching a maximum adsorption capacity of 184.2 mg g^{-1} at pH 5.5. Simultaneously, the material acted as a sensitive optical sensor. Under UV excitation (365 nm), the blue fluorescence (440 nm) was systematically suppressed by Hg^{2+} (Stern-Volmer, R^2 > = 0.994). Selectivity against Pb, Cd, and Cu was confirmed. BioAlg@C-dots represent an innovative dual technology for water resource protection.

Agradecimentos/Acknowledgments

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Synergistic interaction between glass fertilizers and plant growth-promoting microorganisms: beyond conventional nutrition

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Palavras Chave:*Controlled-release fertilizers,PGPM,Nutrient solubilization,Phosphosilicate glass,Food security*

Highlights

Phosphosilicate glasses allow for the controlled release of nutrients.
PGPM strains remain viable even in acidic vitreous extracts.
Cratered surfaces indicate active corrosion and ion exchange.

Resumo/Abstract

According to the International Fertilizer Association (IFA), fertilizers contribute approximately 50% of global food production and are vital for food security. However, in regions like Brazil, nearly 40% of applied fertilizers are lost, highlighting a critical need for innovation in nutrient delivery. In this context, phosphosilicate glass fertilizers have emerged as promising controlled-release materials to enhance nutrient use efficiency. This study proposes an innovative strategy by associating these glasses with plant growth-promoting microorganisms (PGPM). The selected strain (458) is capable of nitrogen (N) fixation and phosphorus (P) solubilization, potentially reducing reliance on synthetic sources and minimizing soil immobilization. Phosphosilicate glasses with a structural P-O-Si framework were synthesized via the melt-quenching method, ground, and sieved (≤ 0.1 mm). Release assays were performed in citrate buffer (pH 4) and ultrapure water over 2 to 64 h, with multielemental quantification via ICP-OES. Bacterial viability in the resulting vitreous leachates was evaluated by counting colony-forming units (CFUs). Data were analyzed using ANOVA and Tukey's test ($p < 0.05$), complemented by chemical and morphological characterization. Initial results confirm the material's controlled-release nature, with rates significantly influenced by the medium. Notably, the ionic concentrations in the leachates did not impair bacterial viability, even at acidic pH. Morphological alterations, including surface precipitation and the formation of "craters," indicate vitreous corrosion and structural changes driven by the material's hygroscopicity. This interaction suggests that the glass-microbe association can modulate release kinetics while supporting microbial life, offering a robust tool for sustainable agriculture.



Controlled-release fertilizer glass in synergy with N-fixing and P-solubilizing bacteria

Agradecimentos/Acknowledgments

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Synthesis and characterization of a methacrylic isocyanate for potential application in the development of methacrylic monomers.

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Palavras Chave:*2-Hydroxyethyl methacrylate,4,4'-Methylenebis(phenyl isocyanate),Methacrylic isocyanate*

Highlights

Sustainable synthesis of a urethane methacrylate using acetone as a safer and greener solvent alternative.

Resumo/Abstract

Photopolymerizable resins have attracted growing industrial interest due to their fast curing, low energy consumption, and application versatility. Aiming to combine the mechanical versatility of urethane linkages with the reactivity of acrylic groups, this work describes the synthesis of an “methacrylic isocyanate” intermediate (MDI-HEMA adduct), designed as a precursor for the future production of a methacrylic monomer from the reaction with renewable polyols. Aligned with principles 3 and 5 of Green Chemistry, the synthetic route substituted toxic solvents, such as dimethylformamide or methylene chloride, with acetone. Characterization by mid-infrared spectroscopy (MIR) indicated the formation of the urethane linkage by the appearance of secondary amide bands (N-H stretching at 3304 cm^{-1} and bending at 1593 cm^{-1}) and confirmed the integrity of the acrylic functionality (C=C at 1639 cm^{-1}), which is fundamental for photopolymerization. The persistence of the band at 2296 cm^{-1} (–N=C=O) suggests the formation of the monoadduct, a hypothesis to be corroborated in the future via ^{1}H-NMR. Ultraviolet-visible spectroscopy (UV-Vis) suggests a possible structural change, as the band with λ_{max} = 298 nm present in the reactant is no longer observed in the product. Conversely, the retention of the band with λ_{max} = 272 nm, attributed to benzene π-π* transitions, indicates the preservation of the aromatic structure. Simultaneous Thermogravimetry-Differential Thermal Analysis (TG/DTG-DTA) revealed that the product has superior thermal stability (153 °C) compared to MDI (115 °C). The adduct presented two mass loss stages (153–379 °C and 380–728 °C), with mass losses of 36.59% and 61.73%, respectively. Additionally, the MDI DTA curve showed an endothermic peak at 56.8 °C, attributed to melting after qualitative tests, an event absent in the final product; furthermore, an exothermic event at 575.6 °C was observed, initially attributed to the degradation of its organic matrix.

Agradecimentos/Acknowledgments

São Paulo Research Foundation - FAPESP (grants 2025/12505-7; 2024/14279-1; 2024/00779-2; 2025/25333-0), National Council for Scientific and Technological Development - CNPq (grant 303968/2024-9), and CAPES (grant 88887.146236/2025-00).

Synthesis and Characterization of Amphiphilic Chitosan Oligomers for mRNA Delivery

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Palavras Chave:*Chitosan, mRNA, Nanoparticles, Gene Therapy, Amphiphilic Polymers*

Highlights

Synthesis/characterization of amphiphilic oligomers with controlled hydrophobicity and charge density.

Precise tuning enables self-assembled nanoparticles with tailored properties.

Resumo/Abstract

Non-viral delivery of messenger RNA (mRNA) has emerged as a promising gene-therapy strategy because it enables transient expression of therapeutic proteins. However, clinical performance depends on safe and efficient delivery systems that protect mRNA from degradation, promote cellular uptake, and facilitate endosomal escape[1]. Here, we propose the synthesis and characterization of amphiphilic polymers designed to form self-assembled nanoparticles for mRNA delivery. Low molecular weight chitosan was functionalized via nucleophilic alkylation with 2-chloroethyl diisopropylethylamine chloride, yielding diisopropylaminoethyl chitosan (CHD) with a targeted degree of substitution of 15%[2]. Subsequently, oxidative depolymerization mediated by sodium nitrite afforded the corresponding oligomer (O-CHD). Finally, N-alkylated derivatives were prepared by reductive amination with octyl aldehyde, followed by reduction with sodium cyanoborohydride. The polymers were characterized by ^{1}H NMR and potentiometric titration. ^{1}H NMR confirmed incorporation of DIPEA moieties (signal at ~1.8 ppm) and n-octyl chains (δ 1.8–1.2 ppm), enabling estimation of the DIPEA substitution degree (13.8%) and verification of controlled octyl substitution (5.3%, 10.0%, 18.5%). Potentiometric titration showed that decreasing molecular weight markedly increased the fraction of protonated groups at neutral pH, from ~20% (CHD) to ~40% (O-CHD), indicating an increased apparent pKa and improved oligomer solubility under physiological conditions. Overall, the resulting polymers are well-suited for RNA complexation and stable nanoparticle development. This synthetic strategy enabled precise control over both polymer charge density and hydrophobicity.

Dowdy SF. Endosomal escape of RNA therapeutics: How do we solve this rate-limiting problem? RNA. 2023;29(5):396–401 Tiera MJ, Fernandes JC, Junior AMM et al. - Chitosan-containing nanoparticles for delivery of polynucleotides, US Patent App. 18/552,321, 2024

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Synthesis and characterization of bimetallic selenium and silver nanoparticles

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Palavras Chave:*Nanotechnology, selenium nanoparticles, Janus nanoparticles, silver nanoparticles.*

Highlights

Synthesis of bimetallic selenium and silver nanoparticles.

Comparison of the individual and synergic properties of the selenium and silver nanoparticles.

High antimicrobial potential and low toxicity.

Resumo/Abstract

Silver nanoparticles have attracted considerable interest in chemistry and physics owing to their high antimicrobial potential and their potential applications in consumer products such as hair products, soaps, and gels. Se nanoparticles are another material that has been increasingly studied, mainly due to their versatility, high biocompatibility, and low toxicity. In addition, selenium aids in the detoxification of metals through selenoproteins that act on liver enzymes, increasing the solubility of silver-containing metabolites and reducing their retention in tissues, which minimizes the systemic adverse effects of this metal. Bimetallic nanoparticles, also known as Janus nanoparticles, are structures with two or more surfaces and different chemical or physical properties. Studies show that Janus nanoparticles composed of selenium and silver have a synergy that increases their antimicrobial potential. Therefore, this work aims to synthesize bimetallic nanoparticles composed of selenium and silver, as well as selenium and silver nanoparticles, through chemical reduction by sodium borohydride ($NaBH_4$), using sodium citrate ($Na_3C_6H_5O_7$) as a stabilizing agent, as well as the characterization of each material through UV - Vis and DLS spectroscopy, comparing their individual and synergic properties in the Janus bimetallic nanoparticles.

Agradecimentos/Acknowledgments

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Synthesis and Characterization of Bio-based Polyamides Derived from Linseed and Pequi Oil Blends.

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Palavras Chave:*Vegetable oil, maleinization, polyamides,Vegetable oil,maleinization,polyamides*

Highlights

Sustainable polyamides with customizable and adjustable luminescent properties.

Resumo/Abstract

The production of petroleum-based polymers has increased significantly owing to their versatility and broad range of applications. Indeed, according to the World Economic Forum, these materials are projected to account for approximately 20% of global petroleum consumption by 2050.Despite their utility, however, their synthesis often releases toxic gases, and the resulting materials are frequently non-recyclable.Driven by these environmental concerns, the use of renewable feedstocks such as vegetable oils has gained significant attention, as these sources offer high availability, low cost, and low toxicity, thereby enabling the development of greener polymeric materials. In this work, polyamides were synthesized from structurally modified blends of linseed and pequi oil. To achieve this, the blends were prepared by varying the mass fraction of linseed oil to 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0. This variation revealed a linear relationship between the mass fraction and the iodine value (g of I2 / 100g of sample). Subsequently, the monomers were obtained through the maleinization of both the blends and pure vegetable oils with maleic anhydride (MA). These resulting monomers exhibited varying degrees of anhydride incorporation, ranging from 5.6 to 17.7 g of MA per 100 g of maleinized oil.To evaluate their properties, both the vegetable oil blends (VOBs) and the maleinized monomers were characterized by Simultaneous Thermogravimetry - Differential Thermal Analysis (TG-DTA). The results indicated that as the degree of unsaturation increased, the thermal stability of the VOBs decreased (ranging from 233.6 °C to 185.5 °C). For the maleinized monomers, thermal stability decreased with increasing anhydride incorporation (from 219.6 °C to 196.5 °C). Finally, these monomers reacted with ethylenediamine to synthesize polyamides. The curing process was conducted at 110 °C, with the conversion rate monitored using Mid-Infrared Spectroscopy (MIR).

Agradecimentos/Acknowledgments

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Synthesis And Characterization of Carbon Dots by a Fast Microwave Route

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Palavras Chave:*Fluorescent nanoparticles, microwave, fast synthetic route, fluorophores*

Highlights

Carbon dots with anexcitation-independent emission were synthesized in a domestic microwave. molecular states influence in emission, fluorophores formation under carbonization

Resumo/Abstract

Since their accidental discovery in 2004, carbon dots (CDs) have been a growing topic over the years. However, only after the discovery of fluorophore formation during its synthesis in the mid-2010s that excitation and fluorescence mechanisms were properly discussed and studied to this day. In this work, we successfully synthesized CDs via domestic microwave under thermal treatment for 30 minutes using citric acid and tris base as reagents. We analyzed two samples, CDs as-synthesized (CDAs) and CDs dialyzed (CDDil.) under a dialysis membrane with a MWCO of 14kDa for 4 days. The carbonaceous material revealed a strong, bright blue fluorescence after suspended in water. DLS analysis of CDAs showed a particle size of around 2-4 nm, as expected for CDs. UV-Vis analysis of CDDil. showed a peak around 330 nm, with a shoulder at 234 nm, being attributed to n-π* transitions at the carbon lattice, and to π-π* transitions of sp2 hybridized carbon, respectively. PL spectra of CDDil. showed a peak at 440 nm, with a narrower FWHM compared to CDAs. Additionally, a dialysate analysis showed a strong presence of molecular states with also excitation-independent emission, with all samples exhibiting a behavior obeying the Kasha-Vavilov rule. FTIR spectra showed a presented a band at 1735 cm-1, assigned to C=O stretching. Furthermore, the band at 1662 cm-1, attributed to to C-N vibration, denotes the presence of those moieties, exposing a structure evolution under synthesis. These results demonstrate that the CDs synthesized have a strong presence of molecular states in their formation, and, even after proper dialysis, the influence of fluorophores on their emission was detected, possibly attached to the carbon-core. The CDs will be further utilized in the development of an analytical sensor based on a microfluidic paper with molecularly imprinted polymers formation, in hopes of being capable of detecting cocaine in seized samples for forensic analysis in a selective way.



Figure 1 - Carbonized material and its bright blue fluorescence after suspension in water

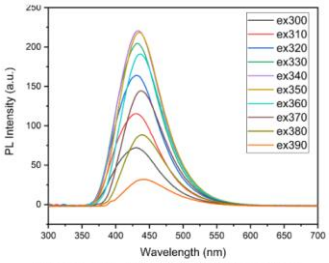


Figure 2 - PL spectra of CDDil.

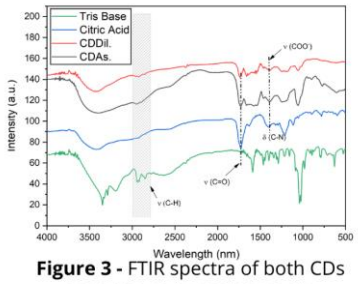


Figure 3 - FTIR spectra of both CDs samples and used reagents

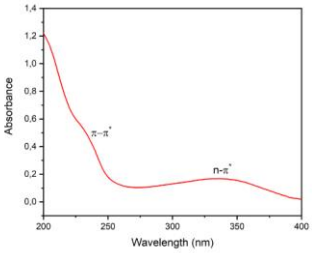


Figure 4 - UV-Vis spectra for CDDII.

Carbonized material and its fluorescence in water, PL, FTIR and UV-VIs spectra, respectively

Agradecimentos/Acknowledgments

Laboratory of Analytical Methods Development (LADEMA), Advanced Functional Materials Laboratory (LAMFA), State University of Londrina (UEL), Brazilian Council for Scientific and Technological Development (CNPq).

Synthesis and Characterization of Cholesterol-Modified Tertiary Amine Oligochitosan Nanocarriers

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Palavras Chave:*Chitosan,siRNA,mRNA,Nanoparticles,Cholesterol*

Highlights

Cholesterol-grafted amphipilic oligochitosan derivates for mRNA delivery pH-responsive formation of polymeric nanoparticles

Resumo/Abstract

Nucleic-acid delivery of siRNA and mRNA is a promising pharmaceutical strategy for vaccines, immunotherapy, and the treatment of infections, cancer, and rare diseases [1]. Its success depends on efficient cationic carriers that enable nucleic-acid complexation, protection, and intracellular release. In this work, low–molecular weight chitosan was functionalized with diethylaminoethyl (DEAE) or diisopropylaminoethyl (DIPEA) groups using the corresponding 2-chloroethyl tertiary-amine reagent under pH control. The products were purified by dialysis and lyophilized. DEAE-CH and DIPEA-CH were then oxidatively depolymerized in 2% (v/v) acetic acid and purified by dialysis and lyophilization to yield O-DEAE-CH and O-DIPEA-CH. Cholesterol was conjugated to O-DEAE-CH and O-DIPEA-CH via EDC/NHS activation in 2% acetic acid, followed by dropwise addition of cholesterol succinate in DMF. Polymers were characterized by ^{1}H NMR (degrees of substitution/acetylation) and potentiometric titration (protonation/ionization behavior). Cholesterol grafting was confirmed, affording O-DIPEA-CH**4**(GS_Chol ≈ 3.9%), O-DIPEA-CH**7**(≈ 7.0%), and O-DEAE-CH**9**(≈ 8.9%). Cholesterol-modified O-DIPEA-CHX formed nanometric siRNA polyplexes: at N/P 10, the hydrodynamic diameter (Dh) decreased from ~250 nm (DIPEA-CH) to ~70–120 nm (O-DIPEA-CH**4**), while ζ-potential remained slightly positive. Particle size depended on pH and N/P (e.g., pH 7.4: ~265 nm for DIPEA-CH vs ~90 nm for the cholesterol derivative at N/P 10). The low-Mw O-DIPEA (~10.2 kDa) showed weak binding (Dh ~1000–1700 nm), whereas ~7% cholesterol (O-DIPEA-CH7) reduced Dh to ~300 nm. Overall, these results demonstrate precise control over oligomer charge density and hydrophobicity, and highlight the role of cholesterol in promoting stable nanometric polyplexes in the ~100–300 nm range.
[1] Shi, Y., Shi, M., Wang, Y. et al. Progress and prospects of mRNA-based drugs in pre-clinical and clinical applications. Sig Transduct Target Ther 9, 322 (2024).

Agradecimentos/Acknowledgments

National Institute of Gene Therapy (CNPq), Grant No. 401811/2024-7; FAPESP, Grants No. 2019/27801-0 and 2023/03182-4

Synthesis and characterization of fluorotungstate-based X-ray scintillators via hydrothermal route

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Palavras Chave:*Scintillators,Fluorotungstates,Hidrotermal synthesis,XEOL*

Highlights

This work reports hydrothermal synthesis of underexplored flurotungstate-based scintillators, by varying time, temperature and reagent concentration, as well as their characterization.

Resumo/Abstract

Scintillators are materials capable of absorbing high-energy radiation and converting it into visible or ultraviolet light. As a result, scintillators have a wide range of applications such as X-ray detection, medical imaging and dosimetry, security measures and high-energy physics.
In this study, barium fluorotungstate ($Ba_2WO_3F_4$) was obtained by reacting $BaWO_4$ with HF whilst in hydrothermal conditions, similarly as described in [1] and [2].
The obtained material was characterized using X-ray diffraction, its morphology was observed with the assistance of a SEM and XEOL was observed via a radioluminescence detector.
The characterization confirmed the formation of $Ba_2WO_3F_4$, consistent with the database ICSD#201653 (Figure 1), its morphology (Figure 2), and demonstrated a peak radioluminescence at 526 nm (green) (Figure 3).
References:
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[2] SRIVASTAVA, A. M.; ACKERMAN, J. F. Synthesis and luminescence of dioxo W6+ (d0) complex: BaWO2F4. Materials Research Bulletin, v. 34, n. 9, p. 1397–1402, jul. 1999.

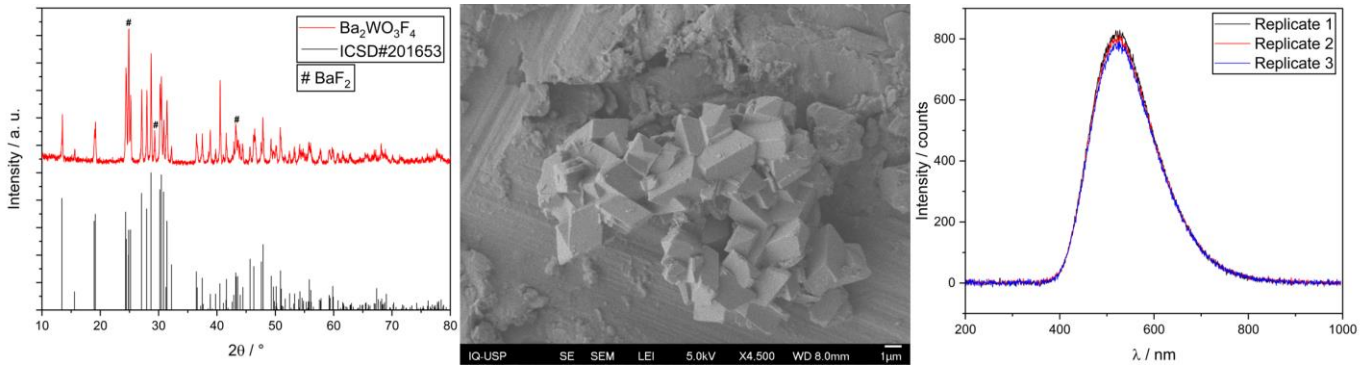


Figure 1: XRD pattern of Ba2WO3F4. Figure 2: SEM of Ba2WO3F4. Figure 3: XEOL spectrum.

Agradecimentos/Acknowledgments

This work was funded by the Programa Unificado de Bolsas (PUB-USP), grant 3662/2025. The authors are grateful to the funding agencies FAPESP and CNPq. Also, to Neilo Trindade and Matheus Nunes of the Institute of Physics - University of São Paulo.

Synthesis and characterization of glasses with magneto-optical properties containing neodymium oxide recovered from discarded electronic materials

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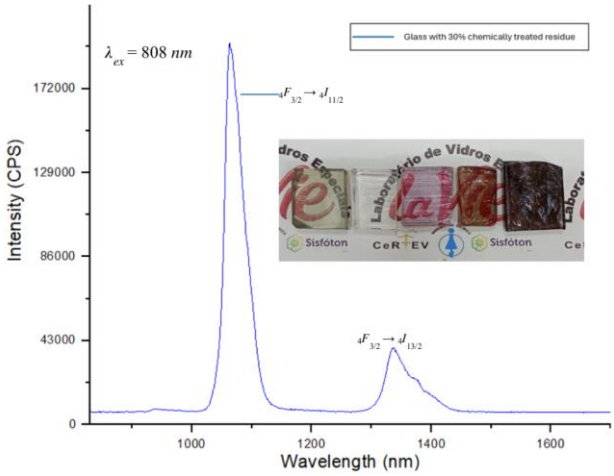
Palavras Chave:*Glasses, Magneto-optical glasses, Rare earth, Electronic waste, Recycle*

Highlights

Borate glasses containing Nd^{3+} ions, obtained from magnets recovered from discarded electronic materials, were synthesized for optical and magneto-optical applications.

Resumo/Abstract

REEs (Rare Earth Elements) such as Nd^{3+} ions are highly applicable for the synthesis of magneto-optical (MO) materials due to their paramagnetic properties. The possibility of recycling rare earth elements found in electronic waste is an interesting alternative for both the economy and the environment. Nd^{3+} has an electronic configuration of $[Xe]4f^3$ and a paramagnetic moment of 3.27 μB. In this work, we synthesized borate glasses containing Nd^{3+} ions obtained from magnets from discarded hard drives. The hard drives were crushed and then leached with 2M hydrochloric acid. Neodymium oxalate was selectively precipitated by adding a 10% oxalic acid solution. In the next step, this neodymium oxalate was calcined to obtain Nd_2O_3. Using Nd_2O_3 obtained, borate glasses based on the BAB-wt%Nd glass composition were synthesized via the melt-quenching method at 1430 °C for 2 hours. All glass samples were analyzed by X-ray diffraction (XRD), differential scanning calorimetry (DSC), and photoluminescence (PL). XRD patterns confirmed the non-crystalline behavior for all samples. From the DSC curves it was possible to extract the glass transition temperatures (Tg) for all samples BAB-0%Nd (at 494ºC); BAB-0.5%Nd (at 496ºC); BAB-5%Nd (at 500ºC); BAB-20%Nd (at 506ºC) and BAB-30%Nd (at 564ºC). The emission spectra of the BAG-xNd glasses, obtained under excitation at 808 nm, presented the typical and electronic transitions at 1062 and 1336 nm, respectively. The preliminary results show synthesis of glass containing neodymium ions opens a range of possibilities for recycling and production of optical and magneto-optical materials.



Synthesized glasses and BAB-30%Nd photoluminescence excitation spectra

Agradecimentos/Acknowledgments

I would like to express my gratitude to Bruno Longhini Machado, Robert Nascimento Mariano, my advisor, Douglas Faza Franco and Elias Paiva Ferreira Neto, my co-advisor, to CAPES, the IQ-Unesp, and the LAVIE and LAMF research groups.

SYNTHESIS AND CHARACTERIZATION OF IRON AND NICKEL SINGLE CRYSTALS FOR MAGNETO-OPTICAL APPLICATIONS

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Palavras Chave:*glass-ceramics, Faraday rotation, magneto-optical, single-crystals, Verdet constant*

Highlights

Glass-ceramic route yields µm-sized Ni^{2+}-doped magneto-optical crystals. Multiple cubic phases coexist. Potential for integrated Faraday rotators in optical sensors.

Resumo/Abstract

Glassy materials containing rare-earth ions enable interesting optical and magneto-optical (MO) applications. The performance of a magneto-optical (MO) material is quantified by a high value of the so-called Verdet constant (V). Manipulating the chemical composition of vitreous materials by adding highly paramagnetic, diamagnetic, or ferromagnetic elements contributes to increased sensitivity regarding the rotation of the light's polarization plane. This work presents the synthesis of Ni-doped single crystals for applications as Faraday rotators. Stoichiometric precursors (PbO, GeO_2, Bi_2O_3, Y_2O_3, Fe_2O_3, NiO) were melt-quenched at 1250 °C and heat-treated to produce a glass-ceramic. Crystals were isolated via concentrated HCl etching. Structural characterization of the extracted crystals was performed using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) coupled with Energy-Dispersive X-ray Spectroscopy (EDS), and Raman Spectroscopy. XRD patterns confirmed the coexistence of cubic phases: magnetite (Fe_3O_4, Fd-3m, a=8.32 Å) and trevorite ($NiFe_2O_4$, Fd-3m, a=8.337 Å). SEM images revealed crystals with sizes of 10–80 µm and varied morphologies, such as hexagons and pyramids. Qualitative EDS analysis confirmed the presence and homogeneous distribution of the main elements Ni, Fe, and Ge. The Raman spectra of the crystals presented the vibrational modes of the T_2g and A_1g at 496 and 680 cm^{-1}, assigned to the trevorite ($NiFe_2O_4$) and magnetite (Fe_3O_4) crystalline phases, respectively. The preliminary results show the successful synthesis of Ni^{2+}-doped single crystals via a glass-ceramic route, indicating promising properties for application as Faraday rotators in integrated MO devices.

Agradecimentos/Acknowledgments

We thank PROPe UNESP, PIBIC/PIBITI for the scholarship and Paulo Research Foundation Agency, FAPESP (grants no 2013/07793-6, 2023/04832-2 and 2025/04339-0) for financial support.

Synthesis and Characterization of Magnetic Nanoparticles for Applications in Electrocatalysis Assisted by Magnetic Field

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Palavras Chave:*Iron oxide magnetic nanoparticles; Cerium doping; Electrocatalysis; Magnetic hyperthermia.*

Highlights

Ce-doped Iron oxide magnetic nanoparticles show enhanced magnetic heating; Ce doping increases saturation magnetization and SAR; Promising material for electrocatalysis assisted by magnetic field.

Resumo/Abstract

Iron oxide magnetic nanoparticles (IOMN), especially magnetite and maghemite, have been widely investigated due to their magnetic properties and their applications in magnetically assisted electrocatalysis processes. The heating capacity of the IOMN under alternating magnetic field (AMF), (magnetic hyperthermia), is important for electrocatalysis assisted by AFM. In this work, IOMN and IOMN doped with 0.1% cerium (IOMN-Ce) were synthesized by the coprecipitation method [1]. X-ray diffraction confirmed the formation of the magnetite or maghemite phase in both samples [1], with average crystallite sizes estimated by the Scherrer equation of ~ 14.50 nm and 14.46 nm for IOMN and IOMN-Ce, respectively. Electron paramagnetic resonance measurements showed g-factors of 2.49 for IOMN and 2.51 for IOMN-Ce, indicating superparamagnetic behavior. The magnetization curves M(H) also evidenced superparamagnetic behavior for both samples, with saturation magnetizations of 46 emu/g for IOMN and 55 emu/g for IOMN-Ce. The higher value of saturation magnetizations of IOMN-Ce suggests better heating capacity under AFM, which is suitable for electrocatalysis assisted by AMF. Magnetic hyperthermia experiments under fields with amplitudes of 16, 22, 30, 40, and 50 mT and frequencies of 988, 628, 445, 260, and 173 kHz provides values of SAR ranging between 104.65 and 128.36 W/g for IOMN, while the IOMN-Ce showed superior performance, with values between 97.75 and 281.94 W/g, with the highest value under the condition of 16 mT and 988 kHz, in addition to a greater ΔT, reaching 47.5 °C within an 80 second interval. The improvement in the hating capacity under the AMF of IOMN doped with Ce agrees with the results obtained by Kowalik et al. [2], which doped IOMN with Y. Thus, the IOMN-Ce is a suitable material for electrocatalysis assisted by AMF.
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[2] Przemyslaw Kowalik, et al. J. Phys. Chem. C**2020**, 124, 6871-6883

Agradecimentos/Acknowledgments

FAPERJ proc. E-26/210.611/2024, CNPq proc. 406354/2025-1 and 300188/2025-0, PIBIC-UFF and CBPF.

Synthesis and evaluation of Ru/LDH catalysts modified with carboxymethyl-β-cyclodextrin for hydrogenation reaction of N Ethylcarbazole

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Palavras Chave:*Hydrogenation,N-ethylcarbazole,Layered Double Hydroxide,Ruthenium Catalysts,Cyclodextrin*

Highlights

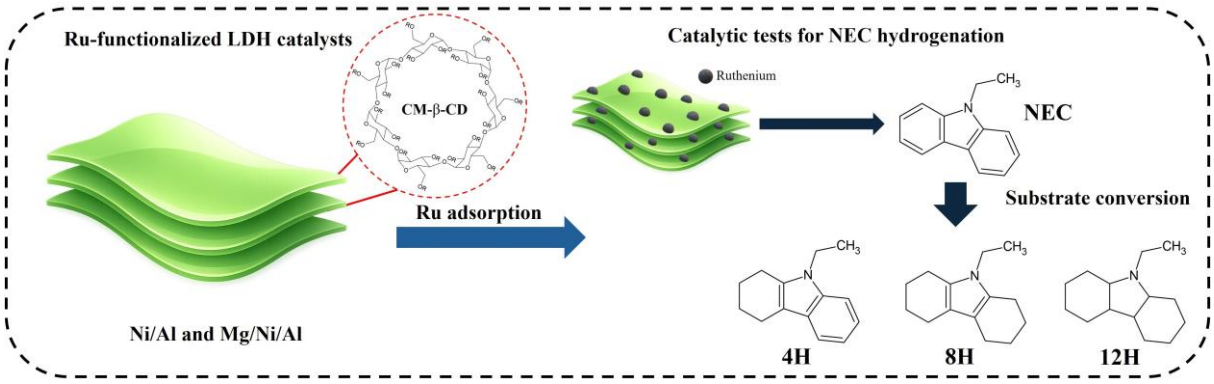
Ru catalysts supported in LDH were developed NEC hydrogenation; Unmodified Ni/Al LDH/Ru matched commercial Ru/Al_2O_3 in activity, but the addition of CM-β-CD in the catalyst decreases its efficiency.

Resumo/Abstract

The increasing demand for safe hydrogen storage has driven research into liquid organic carriers such as N-ethylcarbazole (NEC). However, its catalytic hydrogenation is required for hydrogen storage and demands more efficient catalysts. This work addresses this challenge by developing Ru catalysts supported in layered double hydroxide (LDH), based on Ni/Al systems, modified with carboxymethyl-β-cyclodextrin (CM-β-CD) to enhance metal dispersion. Using XRD, FTIR, XRF, XPS and catalytic test, the study correlates material structure and composition with hydrogenation performance to guide the design of improved catalysts for hydrogen storage applications.

The Ni/Al LDH was synthesized by coprecipitation, then intercalated with CM-β-CD under N_2 for 2 h at room temperature, followed by Ru^{3+} adsorption (reflux, 80 °C, 4 h) and reduction with $NaBH_4$ (reflux, 80 °C, 24 h). Characterization by XRD, FTIR, XRF confirmed structural integrity, organic impregnation (instead of intercalation), and effective Ru incorporation (~1.7-2.3 wt% in Ni/Al systems). Catalytic tests for NEC hydrogenation revealed that Ni/Al LDH with reduced Ru performed equivalently to the commercial Ru/Al_2O_3 benchmark catalyst, both achieving complete substrate conversion. In contrast, CM-β-CD intercalation drastically reduced activity, despite the confirming Ru presence mostly on surface (0.56 at% and ~7 wt% by XPS).

In conclusion, the unmodified Ni/Al LDH with reduced Ru is the most effective catalyst for NEC hydrogenation, performing equally to the commercial Ru/Al_2O_3. This confirms the native LDH structure optimizes Ru activity, providing a key design principle for efficient hydrogen-storage catalysts; however, whatever the role of cyclodextrin it decreased reactivity, probably by inactivation of NEC due to supramolecular complexation; furthermore LDH alone did not exhibit catalytic activity without the supported metal.



Use of CM-β-CD-modified Ru/LDH catalysts in NEC hydrogenation.

Agradecimentos/Acknowledgments

We acknowledge CNPq, FAPERJ and CAPES for funding and Ph.D. Marcelo Huguenin Maia Costa and Ph.D. Suellen Dayenn Tozetti, members of*Department of Physics of The PUC-Rio,*for XPS analyses.

Synthesis and Thin Film Deposition of La-Doped BiFeO3 by Spin Coating: Influence of Rare Earth Doping on Structural Properties

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Palavras Chave:*Thin films, Coprecipitation, Spin coating, Multiferroics,Bismuth ferrite,,Thin films,,Bismuth ferrite,Thin films,Coprecipitation,Spin coating,Multiferroics*

Highlights

BFO/LaBFO powders and thin films were successfully obtained via wet-chemical synthesis

Spin coating enabled good depositions of multilayer BFO/LaBFO thin films

Resumo/Abstract

Multiferroic materials have been investigated because of their key role in the development of advanced technologies, as they exhibit two or more ferroic properties simultaneously, such as ferromagnetism, ferroelectricity, and ferroelasticity. The bismuth ferrite, $BiFeO_3$ (BFO), is a promising multiferroic ceramic. It simultaneously combines ferroelectric and antiferromagnetic properties at room temperature. Moreover, La-doped $BiFeO_3$ has been widely explored as a strategy to enhance structural, electronic and functional properties, making it a good material for applications in memory devices, sensors and photocatalysis processes. This study aims to synthesize pure $BiFeO_3$ and La-doped $BiFeO_3$ powders by the coprecipitation method using bismuth nitrate pentahydrate ($Bi(NO_3)_3.5H_2O$), iron nitrate nonahydrate ($Fe(NO_3)_3.9H_2O$) and lanthanum nitrate as precursor agents, with potassium hydroxide (KOH) as the precipitating agent. The precipitate was then macerated and calcined under a temperature of 550 °C for 3 hours in order to obtain the crystalline phase. The calcined powder was dispersed in a suspension of terpineol and ethylcellulose and then, thin films ranging from 1 to 10 layers were deposited using the spin coating technique on silicon substrates (Si(100)), with post-heat treatment. The characterization of powders and thin films were performed by X-ray diffraction to confirm the formation of pure BFO crystalline phase and to identify the presence of residual secondary phases in doped compounds, The morphology was investigated by SEM-EDS, indicating well-defined particle shapes and a homogeneous elemental distribution, while particle size and zeta potential were analyzed by DLS, indicating an average hydrodynamic diameter in the nanometric range and a stable colloidal dispersion. These results demonstrate the successful incorporation of lanthanum into BiFeO3 and the feasibility of the proposed methodology for producing high-quality multiferroic powders and thin films.

Agradecimentos/Acknowledgments

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Synthesis of Alg@Biochar biobeads from Astrocaryum aculeatum for the efficient removal of Pb^{2+} and Hg^{2+} from industrial effluents

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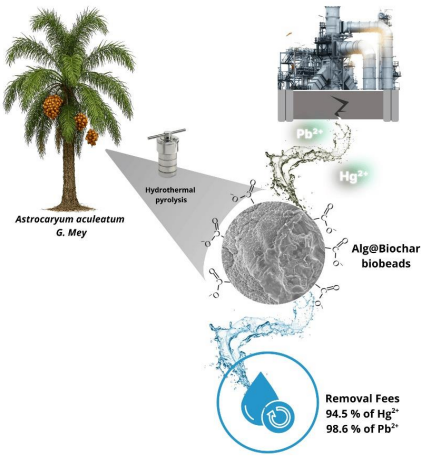
Palavras Chave:*Adsorption, Tucumã Biochar, Alginate Biobeads, Water Remediation, Potentially Toxic Metals*

Highlights

Alginate–biochar biobeads synthesized from Amazonian residues. Alg@Biochar achieved high Hg^{2+} (94.5%) and Pb^{2+} (98.6%) removal efficiency.Sustainable adsorbent for water remediation applications.

Resumo/Abstract

The increasing contamination of water resources by potentially toxic metals poses critical challenges to water security and public health. Given the limitations regarding efficiency and cost of conventional methods, adsorption stands out as a viable and sustainable alternative. This study investigated the synthesis and application of alginate biobeads incorporated with biochar derived from the residual biomass of Astrocaryum aculeatum (tucumã), the Alg@Biochar composite, for the remediation of aqueous systems contaminated by Pb2+ and Hg2+. The biocomposites were prepared via ionotropic gelation and characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and surface area analysis, confirming a favorable morphology and the availability of active sites. Adsorption assays demonstrated that the Alg@Biochar biobeads achieved significant removal efficiencies of 94.5% for Hg2+ and 98.6% for Pb2+. These results are attributed to the synergistic effect between the alginate functional groups and the porous structure of the biochar. The study validates the potential of this material for industrial effluent treatment, aligning high remediation performance with the valorization of Amazonian agro-industrial residues within a circular economy framework.



Alg@Biochar biobeads from Astrocaryum aculeatum for efficient Pb2+ and Hg2+ removal

Agradecimentos/Acknowledgments

The authors thank CMABio-UEA for microscopy Electrochemistry Lab-UFAM for facilities, and CAPES and CNPq for financial support.

Synthesis of core–shell $NaGdF_4$ upconverting nanoparticles via mechanochemistry: A phase-and shape-controlled approach

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Palavras Chave:*: Upconversion, Core-shell, Lanthanide*

Highlights

$NaGdF_4$: YbEr nanoparticles obtained via mechanochemical synthesis with phase control of shape, size and upconversion emission, including core-shell architecture, in a fast and sustainable route

Resumo/Abstract

$NaGdF_4$: YbEr upconversion nanoparticle (UCNP) with hexagonal crystalline phase have been commonly synthesized via thermal decomposition methodology. However, this synthesis method required high temperatures, sometimes long reaction times and organic solvents resulting in an unsustainable methodology. The mechanochemistry methodology arises as an environmentally responsible synthetic route for obtaining UCNP, since it works at room temperature and may eliminates toxic solvents. This work illustrates the preparation of upconversion $NaGd_{0.80}F_4$: $Er_{0.02}Yb_{0.18}$ nanoparticles via high-energy milling, using lanthanide nitrates and surface ligands (sodium oleate and sodium citrate) allowing efficient control of crystalline phase and morphology of the nanoparticles. Furthermore, this methodology can be extended to the preparation of core–shell architectures, in obtaining of $NaGd_{0.80}F_4$: $Er_{0.02}Yb_{0.18}$@$NaGd_{0.75}F_4$: $Nd_{0.25}$ nanoparticle, thereby expanding the potential of these nanomaterials for technological applications. In order to accomplish these characteristics experimental protocols such involving milling time and fluorides to lanthanides molar concentration ratios in the formation of hexagonal crystalline phase were evaluated. The transmission electron microscopy images show spheroidal particles with average size of 15.6 nm. The surface functionalization plays an important role in controlling the crystalline structure. The nanoparticles shows upconversion emissions from the ErIII ion at 520, 545 and 654 nm exciting at 980 nm. These results demonstrate that the mechanochemical approach is an efficient and sustainable strategy for the synthesis of core-shell UCNPs with structural and optical control

Agradecimentos/Acknowledgments

The authors are grateful to CNPq, FAPESP, CAPES, CINE e Shell

Synthesis of hydroxyapatite nanostructures containing different titanium concentrations

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Palavras Chave:*calcium phosphate; adsorption; filters; metals; nanoparticles*

Highlights

Hydroxyapatite nanostructures containing different titanium concentrations have been developed and can possibly be applied to adsorb potentially toxic materials.

Resumo/Abstract

alcium phosphates, particularly hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$), are known for being exceptionally versatile, for acting as reference materials for bone tissue regeneration, and, more recently, for being efficient adsorbents during environmental remediation of potentially toxic metal ions that are present in industrial effluents. The large surface area of HA nanostructures, improved by ionic modification with titanium, may provide pure HA with higher adsorptive potential. Here, we have modified HA nanostructures with 1, 5, or 10% titanium by the chemical co-precipitation method in alkaline medium (pH = 10). We used calcium nitrate [$Ca(NO_3)_2{\cdot}4H_2O$], ammonium phosphate [$(NH_4)_2HPO_4$], and titanium isopropoxide [$Ti(OiPr)_4$] as Ca^{2+}, PO_4^{3-}, and titanium source, respectively. The $Ca(NO_3)_2$ and $Ti(OiPr)_4$ solutions were homogenized; next, an $(NH_4)_2HPO_4$ solution was added dropwise, under stirring. X-ray diffraction (XRD) analysis (Fig. 1a) confirmed that pure HA and HA containing 1 or 5% titanium displayed peaks at 2θ = 25.8°, 31.8°, and 32.9°, due to the HA phase (hexagonal cell, PDF 89-6439); no secondary phases were detected. HA containing 10% titanium displayed additional peaks at 2θ ≈ 27.4° and 36.1°, attributed to the rutile phase (TiO_2, PDF 89-0552), which evidenced excess titanium. Transmission electron microscopy (TEM, Fig. 1 b) revealed nanometric porous particles, which increase the adsorption capcity as compared to pure HA.

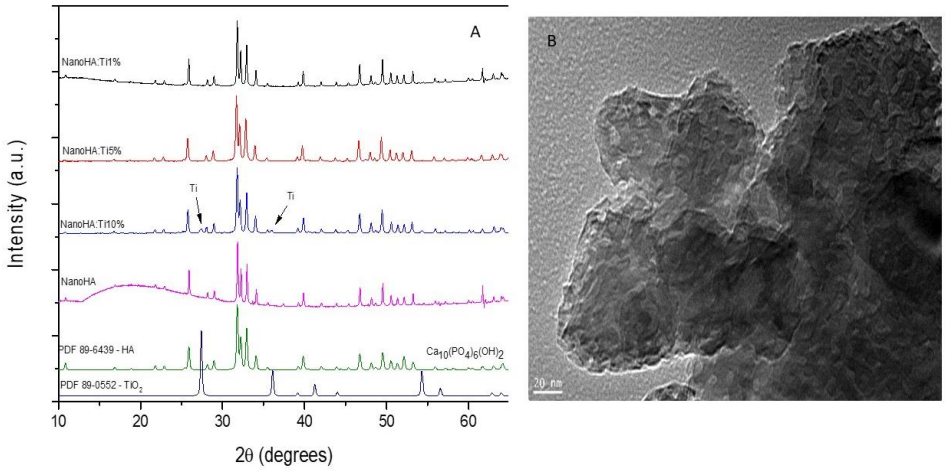


Figure 1: a) X-ray diffractograms of pure hydroxyapatite (HA) and HA doped titanium b) SEM HA.

Agradecimentos/Acknowledgments

CAPES, CNPq, and FAPESP

Synthesis of luminescent materials based on Lithium Antimonate

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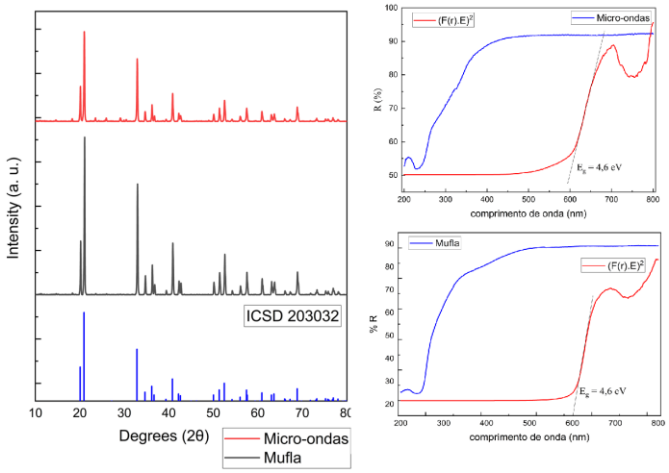
Palavras Chave:*microwave-assisted solid-state synthesis,luminescence,lithium antimonate*

Highlights

Study of the interference of synthesis parameters of crystalline $LiSbO_3$ nanostructures by the microwave-assisted solid-state method.

Resumo/Abstract

We report the synthesis of crystalline LiSbO3 nanostructures using a microwave-assisted solid-state method, where the material was obtained as a single phase (ICSD 203032) in just 30 minutes. Conventional synthesis methods for these materials involve solid-state reactions, which require extremely high temperatures for long periods, resulting in significant energy consumption. The microwave-assisted reaction can reach these high temperatures, but the reaction time decreases considerably. The formation of the desired phase occurs in 30 minutes of reaction with the apparatus operating at 720W 2.45 GHz and iron(III) oxide as a microwave susceptor. At other power levels and reaction times, the formation of other lithium antimonate phases occurs, mainly Li3SbO4.



Diffraction pattern of LiSbO3 synthesized by microwave (red) and the conventional route.

Agradecimentos/Acknowledgments

We would like to acknowledge Capes(153812/2025-00), CNPq, FAPESP and USP.

Synthesis of mesoporous sílica with low-value commercial sand applied to CO2 capture

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Palavras Chave:*Mesoporous, Carbon Dioxide, Surface area, Materials, Characterization*

Highlights

Low-value sand converted into hexagonally ordered mesoporous silica (1204 $m^2 g^{-1}$) exhibiting efficient CO_2 capture performance.

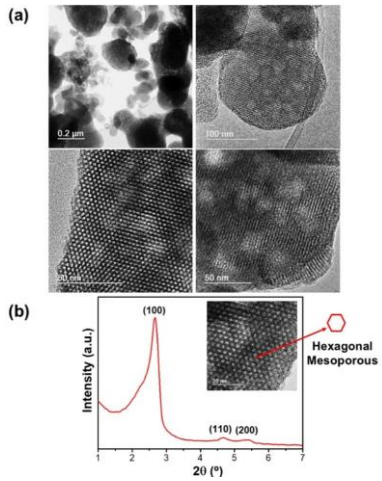
Resumo/Abstract

The increasing atmospheric concentration of CO_2, projected to reach 425.7 ppm in 2025, reinforces the urgency of developing efficient carbon capture technologies. In this context, porous solid adsorbents emerge as promising alternatives to conventional amine-based systems. This work reports the synthesis of mesoporous silica (MCM-41) using low-value commercial sand as an alternative silicon source, replacing tetraethyl orthosilicate (TEOS).

Sodium silicate was obtained from sand via alkaline hydrothermal treatment at 200 °C for 8 h using NaOH solution and subsequently employed in the precipitation synthesis of mesoporous silica using CTAB as a structure-directing agent at room temperature with pH adjusted to 9. After calcination at 540 °C, the material exhibited a highly ordered hexagonal mesoporous structure, confirmed by low-angle XRD and TEM. Nitrogen adsorption–desorption analysis revealed a high specific surface area (1204 $m^2 g^{-1}$), total pore volume of 0.79 $cm^3 g^{-1}$, and average pore diameter of 3.85 nm, characteristic of MCM-41-type materials.

CO_2 adsorption tests performed at 0, 10, and 25 °C up to 1 bar showed maximum capacities of 1.57, 1.51, and 0.82 mmol g^{-1}, respectively, indicating an exothermic physisorption process. At 10 °C, the material demonstrated high CO_2/N_2 selectivity (up to 93 at low pressures) and good stability over six adsorption–desorption cycles, maintaining approximately 88% of its initial capacity. Experimental data showed excellent fitting to both Langmuir and Freundlich models ($R^2 > 0.999$), with $n > 1$ suggesting favorable adsorption.

These results demonstrate that low-cost commercial sand can be successfully valorized into high-performance mesoporous silica for CO_2 capture, offering a simplified and economically attractive synthesis route with potential for sustainable industrial applications.



TEM image (a) and low-angle X-ray diffraction pattern of the SiO2 sample (b).

Agradecimentos/Acknowledgments

CNPq, Fapemig, Capes, UFMG, Fundep, postgraduate program in chemistry UFMG, chemistry department of UFMG, GruTAm, INCT Midas, LABPEMOL.

Synthesis of nanocomposites of MgHCF, carbon nanotubes, and folic acid for application in targeted cancer treatment.

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Palavras Chave:*Nanocomposites,Cancer treatment*

Highlights

MgHCF nanocomposites, nanotubes, and folic acid emerge as a new strategy against cancer. The study investigates the synthesis of these materials to develop more precise and innovative treatments.

Resumo/Abstract

Cancer is one of the most common diseases and one of the leading causes of mortality. Conventional treatments, such as radiotherapy and chemotherapy, have limitations due to damage to healthy cells and the development of tumor resistance. In this context, nanocomposites stand out as efficient drug delivery systems because they exhibit reduced toxicity, improved targeting, and enhanced cellular internalization.

In this work, three syntheses were carried out using the coprecipitation method: MgHCF, MgHCF/CNTf, and MgHCF/FA/CNTf. The procedure involved mixing a 10 mM solution of magnesium acetate in ethanol (Solution A) with an aqueous solution containing 10 mM ferrocyanide and 40 mM potassium acetate (Solution B), maintained under stirring at 60 °C for 24 h, followed by centrifugation and drying in a muffle furnace.

The formation of the materials was confirmed by XRD, which showed a cubic crystalline structure with intense main peaks at 2θ = 17°, 25°, and 35.5°. SEM images indicated that pure MgHCF exhibits uniform cubic particles, while the incorporation of carbon nanotubes and folic acid altered the morphology to a predominantly rectangular shape, with nanotubes located between the particles. Infrared and Raman spectra revealed the characteristic presence of the C≡N group at approximately 2100 cm^{-1} and the metal–carbon vibration around 500 cm^{-1}. In the Raman spectra, the D, G, and 2D bands of the nanotubes were also observed at 1340 cm^{-1}, 1590 cm^{-1}, and 2700 cm^{-1}. The characterizations confirmed the formation and functionalization of the materials, indicating promising features for future applications in cancer treatment.

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Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG, INCT Nanocarbono, Instituto de Química – UFU, Universidade Federal de Uberlândia, INCT
TeraNano.

Synthesis of ZnAl2O4 via biopolymer-assisted soft-template route and evaluation of its surface properties for methylene blue adsorption

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Palavras Chave:*spinel,adsorption,methylene blue,soft-template,cornstarch*

Highlights

Influence of zeta potential and ultrasonic treatment on surface properties and adsorption performance of ZnAl2O4 synthesized via corn starch soft-template

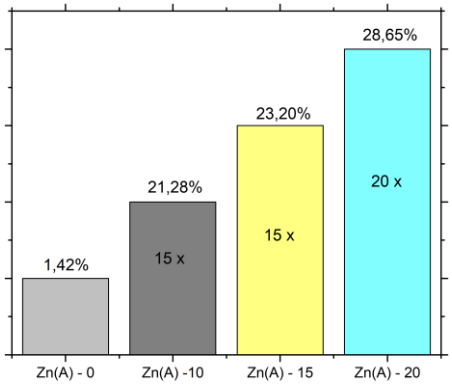
Resumo/Abstract

Several studies have focused on the development of new materials that combine high performance, low cost, and ease of synthesis. In this work, $ZnAl_2O_4$ was synthesized following the methodology proposed by Battiston*et al.*[2], using corn starch as a soft template and subsequently subjected to different ultrasonic treatment times. X-ray diffraction (XRD) confirmed the formation of the spinel-type crystalline phase, which was corroborated by FTIR spectra. The zeta potential measurements showed positive surface charges in the pH range of 2–8, with increasing magnitude at lower pH values and a point of zero charge (PZC) around pH 8. Optical analysis revealed a band gap of approximately 5.51 eV, characteristic of wide band gap semiconductors or insulating materials, with no significant changes after ultrasonic treatment. Scanning electron microscopy (SEM) indicated that $ZnAl_2O_4$presents a porous and sponge-like morphology, attributed to the removal of the starch template. The adsorptive performance of $ZnAl_2O_4$was evaluated through the removal of methylene blue (MB) from aqueous solution at pH 10, a condition that favors electrostatic attraction due to the negative surface charge. After 150 min, the material showed a low removal efficiency (1.42%) at natural pH, whereas at pH 10 a significant increase in MB removal was observed, enhanced by both ultrasonication time and solution pH (Figure 1). These findings indicate that adsorption is mainly governed by the surface chemical properties, being further improved by particle fragmentation induced by ultrasonic treatment.

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Adsorptive performance

Agradecimentos/Acknowledgments

The authors acknowledge the Universidade Estadual de Goiás/Pró-Projetos, the Center for Analysis, Innovation and Technology in Natural and Applied Sciences at UEG (CAiTEC), FAPEG, FINEP, and the IF Goiano for institutional support and infrastructure.

Synthetic control knobs for step-growth polymers and adhesive networks: from low-Đ polyurethanes to switchable and pressure-sensitive adhesives

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Palavras Chave:*polyurethane,pressure-sensitive adhesives,polymerization,covalent-adaptable networks,self-assembly*

Highlights

ADBP adds MW control to step-growth PU (low Đ), sharpening microphase separation and strength. PSA tack/peel is tuned by diisocyanate symmetry, polyol design, crystallinity, and tackifier.

Resumo/Abstract

Step-growth polymerization (SGP) is industrially dominant for polyurethanes (PU) and many networks, yet its intrinsic lack of molecular-weight control (high dispersity, Đ) limits nanostructure definition and, ultimately, performance. Here we show three complementary contributions that connect synthetic precision to phase behavior and macroscopic properties. (1) We discovered a base-triggered thiol/vinyl ether addition that is orthogonal to base-catalyzed thiol–acrylate chemistry, enabling a modular two-stage sequence (acrylate first, vinyl ether end-capping; then UV thiol–ene) to build well-defined phase-separated thermo-switchable adhesive networks. By programming crosslink topology, interphase density, and reversible softening above the switching temperature, the approach delivers improved adhesion and debonding-on-demand. (2) In an ongoing study, we establish a structure–property map for PU pressure-sensitive adhesives (PSAs) by systematically varying polyol functionality and molar mass, diisocyanate symmetry (Figure 1A), hard/soft segment balance, introduction of semicrystalline domains as physical reinforcements, and tackifier identity/loading. Correlating Tg, microphase separation, crystallinity, and the viscoelastic window with tack/peel/shear reveals actionable design rules for high-performance PSAs, including routes to on-demand debondable adhesive systems. Figure 1A highlights how symmetric vs asymmetric diisocyanates tune hard-segment packing and domain purity, shifting the PSA window. (3) Finally, we introduced asymmetric dynamic bond mediated polymerization (ADBP) to decouple growth stages in SGP through selective, reversible bond exchange, yielding polyurethanes with low dispersity (Đ down to ~1.2) at intermediate molar mass. The low Đ enhances microphase-separated ordering and long-range domain coherence, which translates into thermosets with superior mechanical performance and improved structure–property predictability (Figure 1B).

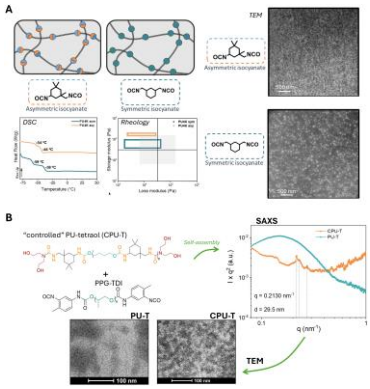


Figure 1. A) Diisocyanate symmetry tunes PU-PSA response. B) ADBP gives low-Đ hard blocks.

Agradecimentos/Acknowledgments

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L.P.F. thanks the ADAGIO

Tailoring the Mechanical and Morphological Properties of Ultralight Nanocellulose Cryogels for Environmental Remediation

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Palavras Chave:*Biomass-based porous material,Cellulosic nanofibrils,Mechanical properties,Natural rubber latex,Freeze-drying*

Highlights

CNF-based composite cryogels obtained from sugarcane bagasse.

Investigation of effect of NR and solid content on cryogel properties.

Property modulation aimed at environmental remediation.

Resumo/Abstract

Cellulosic nanostructures have been widely investigated due to their renewability, low toxicity, high mechanical strength, and large specific surface area, enabling applications as sustainable alternatives to petroleum-derived materials. Porous materials based on cellulose nanofibrils (CNF) can be applied in remediation of oil spills and other hydrophobic contaminants in aquatic environments. However, cellulose is a hydrophilic material, exhibiting low resistance in water. In this context, this work investigates the development of CNF-based cryogels and composite cryogels incorporating natural rubber (NR) latex, aiming to enhance water resistance and tailor mechanical properties. Both systems were prepared with different solid contents, up to 2 wt%. CNF were obtained from sugarcane bagasse, which was initially washed, followed by alkaline treatment with NaOH and two bleaching steps using NaOH and H_2O_2, with procedures adapted from the literature. Mechanical fibrillation was performed by friction using a Masuko Sangyo grinder. Atomic Force Microscopy (AFM) characterization confirmed the nanoscale morphology of the CNF. To obtain cryogels, CNF dispersions were homogenized, cast into cylindrical molds, frozen, and freeze-dried. Mechanical testing revealed a reduction in Young's modulus for NR/CNF cryogels relative to CNF cryogels, indicating a softer material, which is attributed to the elastomeric behavior of NR. X-ray microcomputed tomography (μCT) revealed an interconnected highly porous structure, with a total percentage porosity between 87% and 99%, depending on the solids content. Overall, the incorporation of NR and the control of solid content are shown to be effective strategies for tuning the mechanical and structural properties of cryogels, expanding the range of potential applications in environmental remediation.

Agradecimentos/Acknowledgments

The authors thank the CNPq (Grant No. 303621/2022-2) and FAPESP through the CEPID CEMol program (Grant No. 2024/00989-7) and through the Regular Projects (Grants No. 2025/19844-1 and 2024/21240-4) for financial support.

Targeted biodegradable fluorescent silica nanoparticles for stimuli-responsive release of reactive oxygen and nitrogen species in tumor cells

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Palavras Chave:*Cancer, Photodynamic Therapy, Fluorescent Silica Nanoparticles, Reactive Oxygen Species*

Highlights

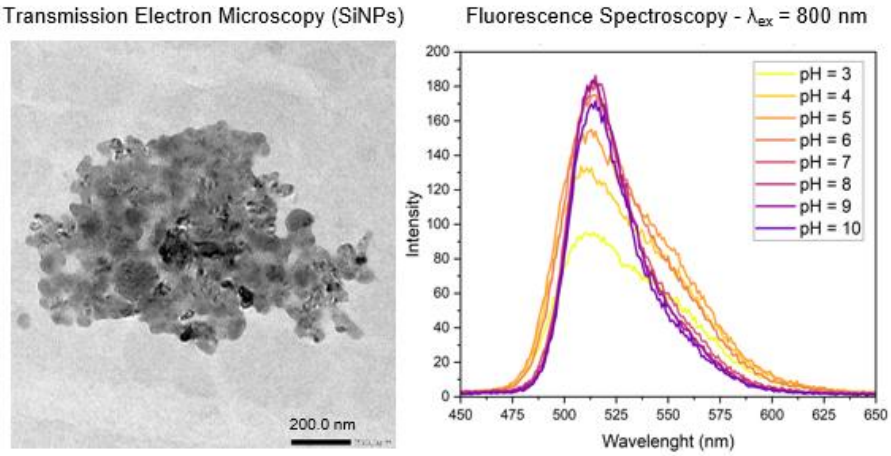
Synthesis of silica nanoparticles in accordance with green chemistry principles.

Material with upconversion properties for enhanced PDT, a selective, minimally invasive, antitumor treatment.

Resumo/Abstract

Cancer mortality remains a critical global challenge, with annual incidence projected to reach 30.9 million cases by 2045. In this context, Photodynamic Therapy (PDT) has gained significant interest as a minimally invasive and selective alternative for tumor treatment, relying on the interaction of light, oxygen and a photosensitizer to produce cytotoxic reactive oxygen species (ROS). The fluorescent silica nanoparticles (SiNPs) synthesized in this project aim to mark their biological location and, in response to radioactive stimuli, promote the release of nitric oxide (NO) by coupled ruthenium complexes, with the objective of enhancing antitumor therapy via ROS. The SiNPs were obtained from a precursor solution of 3-aminopropyltriethoxysilane (APTES) and an aqueous solution of sodium fluorescein (FS). This mixture underwent microwave dielectric heating and was subsequently purified via dialysis1. The purified aqueous SiNPs solution was then used to investigate its physical and optical properties. Transmission Electron Microscopy (TEM) revealed the variety of sizes and morphology of the formed particles. Spectrophotometric analysis (absorbance and fluorescence) showed radioemission identical to FS, indicating its encapsulation by silica, and demonstrated upconversion capability. When excited at 800 nm, the nanoparticles showed luminescence at wavelength at 515 nm. The fluorescence and upconversion capability are present across various pH levels (3-10), with greater intensity in alkaline solutions. These characteristics demonstrate the promising potential of SiNPs for biomedical applications in PDT. The SiNPs are biocompatible, strongly fluorescent, and pH-stable. Future stages of this work involve attaching ruthenium complexes to the external structure of the nanomaterial and investigating the energy transfer processes between the SiNPs and the complexes to optimize their performance as a source for PDT.

[1] https://doi.org/10.1039/C8CC07340F



Transmission Electron Microscopy and Upconversion Capability by Fluorescence Spectroscopy of SiNPs

Textural properties of KOH-Activated Carbon produced from Sugarcane Bagasse

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Palavras Chave:*Activated carbon,Pores,Physisorption*

Highlights

• Activated carbon with high specific surface area value;
• Activated carbon with high micropore volume value.

Resumo/Abstract

In the last century, the populational growth demanded a great industrial development wich led to huge amounts of waste that are hazardous to the environment. One solution for removing these contaminants is adsorbing them with activated carbon.

In order to use it for adsorption, the activated carbon was produced from the biomass of sugarcane bagasse with Potassium Hydroxide (KOH) in three different carbon-to-KOH mass ratios, AC1(1:3), AC2(1:4), and AC3(1:5), evaluating their textural properties looking for the more advantageous ratio for this purpose. Among these properties, some of the most relevant are the specific surface area (SBET) and micropore volume (Vμ), wich were obtained by N_2 physisorption. The pore size distributions (PSD) were obtained according to the equilibrium model of density functional theory. The total pore volumes (VT) were defined as the total amount of N_2 adsorbed at p/p_0 = 0.99, the average pore sizes (APS) were calculated according to the ratio 4SBET/VT, and the micropore volumes (Vμ) were calculated using the t-plot method.

The isotherms shown in Fig. 1(a) are similar to reversible type 1b, showing no hystheresis. It is seen that AC2 is the material that absorbs the most. In the PSD in Fig. 1(b), it is noted that the majority of pores are less than 2.0 nm width, therefore, micropores, the most relevant size of pores in terms of adsorption. Analyzing the textural properties of AC1, AC2, and AC3 the SBET values were 1320, 1642, and 1487m²/g, while Vμvalues were equal to 0.5357, 0.7277, and 0.6108 cm³/g, respectively. Additionally, the APS of such materials were 2.228, 2.035, and 2.214 nm, showing the materials present an structure with mostly micropores. The results showed that among the three materials, AC2 has a greater micropore volume, leading to a greater SBET, wich is some of the most important characteristics in the matter of adsorption, thus, the 1:4 carbon-to-KOH mass ratio is the most favorable one for adsorption technology.

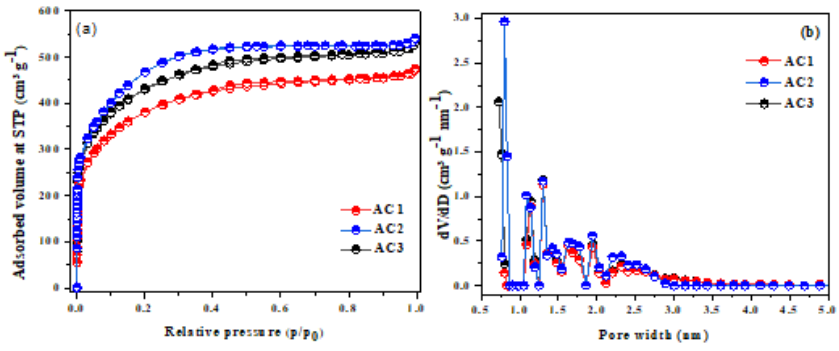


Figure 1. (a) N2 physisorption at 77 K; (b) NLDFT pore size distribution.

Agradecimentos/Acknowledgments

We acknowledge the financial support provided by CNPq and CAPES and for the structure and resources provided by COMCAP, DQI/UEM.

Thin Film Deposition by Magnetron Sputtering Using Solid-State Synthesized Pure and La-Doped BiFeO3 Targets

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Palavras Chave:*Multiferroic, Solid-state, BiFeO3, Sputtering, Thin Film,Multiferroic,Solid-state,, BiFeO3,BiFeO3,Sputtering,Thin Film*

Highlights

Successful synthesis of pure and La-doped $BiFeO_3$ ceramics with well-defined multiferroic phases. High-quality $BiFeO_3$ thin films deposited on Si(100) via RF magnetron sputtering.

Resumo/Abstract

Multiferroic materials are a unique class of functional materials that simultaneously exhibit more than one ferroic order, such as ferroelectricity, ferromagnetism, and ferroelasticity, in a single phase. Among these materials, bismuth ferrite ($BiFeO_3$ - BFO), has attracted significant attention due to its coexistence of ferroelectric and antiferromagnetic ordering at room temperature. Lanthanum doping has been widely explored as an effective strategy to improve phase stability, reduce bismuth volatilization, and enhance the structural, electrical and piezoelectrical properties of BFO. In this work, pure $BiFeO_3$ and 15% La-doped $BiFeO_3$ were synthesized via solid-state route using Bi_2O_3 and Fe_2O_3 as precursor oxides. Stoichiometric mixtures, with a controlled excess of 5% of bismuth, to minimize secondary phases and compensate for volatilization during thermal treatment, were homogenized by mechanical mixing in a mortar and calcined at around 800 °C in order to promote the formation of their respective pure phases. The calcined powders were uniaxially pressed into ceramic pellets and sintered in a resistive furnace to obtain dense ceramics suitable for use as targets in magnetron sputtering for deposition of thin films on a silicon substrate Si(100). Characterization of powders, pellets, and thin films was performed by X-ray diffractometry, scanning electron microscopy (SEM-EDS), and atomic force microscopy to confirm phase formation, crystallinity, particle morphology, and thin-film surface quality. The results demonstrated successful phase formation in the sintered ceramic targets, and in the thin films. SEM-EDS and AFM observations indicated that the sputtered films exhibit smooth surface and microstructural uniformity with homogeneous distribution of the multiferroic thin films. These results indicate that the processing and sputtering deposition methodology were effective and reproducible for the fabrication of high-quality $BiFeO_3$ thin films on silicon substrates.

Agradecimentos/Acknowledgments

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TiO_2–Prussian Blue and Analog Composites: Preliminary Photocatalytic Degradation of Methylene Blue in Aqueous Solution

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Palavras Chave:*Prussian Blue,TiO2,Composites,photocatalysis*

Highlights

Heterojunctions between TiO_2 and Prussian Blue analogs improve photocatalytic efficiency under light irradiation.

Resumo/Abstract

Anatase TiO_2 was coupled to Prussian Blue (Fe–Fe) and cobalt PBAs (Co–Co, Fe–Co, Co–Fe) to probe interfacial redox mediation during methylene blue photodecolorization (MB, 5 ppm, pH 5.6), where MB is mainly the methylthioninium monomer (MB^+) with a minor dimer fraction. XRD/Rietveld confirms anatase and cubic PB/PBA frameworks, with no detectable crystalline Fe–O byproducts. ^{57}Fe Mössbauer (80 K) shows mixed-valence FeII/FeIII in PB (retained in TiO_2/Fe–Fe), low-spin FeII in Fe–Co, and Fe(III)-rich Co–Fe, which splits into two Fe populations upon TiO_2 anchoring, evidencing interfacial electronic heterogeneity. DRS/Tauc gives TiO2-like Eg (~3.2–3.3 eV) for composites plus sub-gap transitions (~1.6–2.0 eV), so rate gains are not driven by band-gap narrowing; SBET trends indicate adsorption/accessibility also contributes. Argon purge lowers decolorization by ~50%, implicating O_2 as the terminal electron acceptor and supporting a mechanism in which PB/PBAs act as electron sinks/redox buffers (PB↔PW; CoIII/CoII), boosting O_2•−/HO_2• while TiO_2 holes generate •OH. TOC removal remains low (~7%), indicating partial transformation; therefore, bee assays (*Scaptotrigona postica*) were included. Kaplan–Meier shows global differences (p=0.0056); pairwise-corrected/Cox analyses (consumption as covariate) are consistent with TL_{50}: C=16 d > E2=12 d > E1=11 d (E2 improves vs E1, not vs C).

Tracking the Eco-Corona Molecular Composition from Soil Dissolved Organic Matter on CuO Nanoparticles Over Time

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Palavras Chave:*Environmental corona,Amazonian Dark Earth,environmental nanotechnology,FT-ICR-MS*

Highlights

- Interaction time regulates competitive molecular binding.

- CHON compounds dominate eco-corona composition.

Resumo/Abstract

Soil is one of the most complex and active environments, and the composition of soil carbon varies across regions and climate conditions, influencing its quality, quantity, lability, and stability profile. The soil dissolved organic matter (DOM) is obtained through water extraction and is the most dynamic and reactive fraction of soil organic matter. Interactions between nanoparticles and soil organic matter occur due to intentional environmental applications, such as the development of new agrochemicals, as well as through natural release, considering their widespread use in various commercial sectors. For agrochemicals, understanding how soil organic composition can modulate eco-corona formation is crucial for enhancing nanomaterial efficiency, minimizing side effects, and predicting the processes and interactions that drive their fate in the environment. Given the highly dynamic and medium-dependent nature of nanoparticle-biomolecule interactions, what can be expected from environments with greater biomolecular diversity, such as soils? What types of molecules will preferentially bind to nanoparticles forming eco-corona? In this work, soil DOM was used to evaluate the eco-corona formation onto copper oxide nanoparticles over time, and both Fourier transform ion cyclotron resonance mass spectrometry and ^{1}H nuclear magnetic resonance was used to monitor compositional changes on soil DOM before and after the eco-corona formation. Although eco-corona composition is highly dynamic and kinetically controlled by the competitive adsorption and desorption of molecules, CHON compounds were the main contributors to the eco-corona composition. Further, interaction time demonstrated to be a relevant parameter affecting eco-corona composition and the equilibrium between bound and unbounded molecules. It promotes intermolecular competition and enables lower-abundance species with higher binding affinities to attach the nanoparticle surface, thereby modulating the eco-corona.

Agradecimentos/Acknowledgments

This study was financed, in part, by FAPESP (2024/18015-9). D.S.T.M. is grateful for the CNPq research productivity scholarship. The authors are grateful to Dr. Aleksander W. Muniz and to Dra. Tsai S. Miu for their assistance with ADE soil sampling.

Tracking the Oxidative-Degradation of Silver Functionalized Graphene Oxide

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Palavras Chave:*Nanothecnology,Nanomaterials,Nanohybrid,Transformation*

Highlights

- NaClO attack GO and AgNPs structures;

- Materials' size decreased during the degradation reaction;

Resumo/Abstract

Graphene oxide decorated with silver nanoparticles (GO-AgNPs) is a widely used material in several areas. However, its transformation during the life cycle remains poorly understood, which is mandatory for safe-by-design approaches (SbD). These strategies focus on minimizing hazards, decreasing bio-persistence and harmful effects. Here, we investigate the chemical degradation of GO-AgNPs induced by commercial NaClO and monitored using several characterization techniques. During the degradation three aliquots were collected to track the changs after 1 day (1D), 5 days (5D), and 10 days (10D). In UV-Vis spectrum, it is possible to observe a characteristics peak at 230 nm and 420 nm associated with π→π* transitions of GO and AgNPs*plasmon*resonance, respectively. However, all long the degradation reaction a significant decay in the peaks' absorbance were presented, followed by a shift from 420 nm to 287 nm of NPs peak, suggesting decreasing the size and surfaces oxidation. Different functional groups (i.e., C-OH, C-O-C, C=O, and COOH) were identified by FTIR (Fourier transform infrared spectroscopy) and XPS (X-ray photoelectron microscopy) for all samples, highlighting the increase in carboxylic content over degradation time due to the oxidation of alcohols into C=O/COOH moieties. Transmission electron microscopy (TEM) and atomic force microscopy (AFM) reveal a significant decrease in NPs size, from 17.05 ± 6.55 nm to 6.84 ± 2.03 nm, followed by GO flakes decreases from 270.95 ± 169.99 nm to 126.55 ± 93.66 nm, for GO-AgNPs and 10D samples, inferring the NaClO attack against GO and AgNPs. Additionally, agglomerated regions were observed in microscopy images, induced by the decrease in nanomaterials' stability and changes in zeta potential 34.63 ± 1.68 mV for GO-AgNPs to -24.09 ± 0.28 mV for 10D, leading to material-material interactions. Therefore, this study provides crucial insights into a nanohybrid's life cycle, contributing to SbD.

Agradecimentos/Acknowledgments

This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Number #2023/13630-4. The authors are grateful to LNNano/CNPEM facilities (XPS, AFM, TEM).

Tricomponent nanocomposite thin films based on conducting polymers (PAni), gold nanoparticles, and molybdenum disulfide.

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Palavras Chave:*Conductive Polymer, Nanocomposites, Tricomponent, Lamellar Materials*

Highlights

Preparation of tricomponent thin films of nanocomposites between conducting polymers, gold nanoparticles, and molybdenum disulfide using the liquid–liquid interfacial route.

Resumo/Abstract

The development of hybrid materials has emerged as a promising strategy for obtaining systems with synergistic and multifunctional properties, especially in electronic, catalytic, and electrochemical applications. Gold nanoparticles (AuNPs) have been extensively investigated due to the strong dependence of their optical, electronic, and catalytic properties on size. One of their most striking characteristics is localized surface plasmon resonance, responsible for intense absorption bands in the visible region. Molybdenum disulfide (MoS_2) is one of the main materials belonging to the transition metal dichalcogenide (TMD) family, standing out for its low toxicity and unique optical properties. Its structure consists of two hexagonal planes of sulfur atoms surrounding an intermediate plane of molybdenum atoms. Polyaniline (PAni) is one of the most widely used conductive polymers due to its simple polymerization, stable material, and doping through protonation. This work proposes the integration of these three materials through the synthesis of three-component thin films using the liquid-liquid interfacial route. This methodology allows the spontaneous formation of films at the interface between two immiscible liquids in a single step1. The twophase system consisted of an aqueous phase containing H_2SO_4 and an organic phase consisting of toluene, with samples obtained with different molar ratios and reaction times. All samples were characterized by X-ray diffraction (XRD), scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS), UV-VIS spectroscopy, voltammetry, and Raman spectroscopy. The variation in the molar ratio between the materials and the different reaction times in the PAni/AuNPs/MoS2 system resulted in modifications in the amount of polymer formed and in the size of the gold nanoparticles in each sample, allowing us to infer potential applications of the films obtained.[1] Zarbin, A. J. G. Mater. Horiz. 2021, v. 8, p. 1409.

Agradecimentos/Acknowledgments

CNPq, CAPES, INCT NanoVida, INCT Nanocarbono and UFPR Scientific and Technological Initiation Coordination.

Tuning Interfacial Interactions in GO@PANI Nanohybrids by Mass Ratio Control

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Palavras Chave:*Nanohybrids,Graphene,Raman Spectroscopy,Polyaniline*

Highlights

A multifunctional nanohybride GO@PANI integrates nanoscale components with enhanced performance.

The nanohybride GO@PANI system shows tunable properties and superior efficiency for advanced materials

Resumo/Abstract

The development of functional materials for applications in energy, sensors, and optoelectronic devices relies on precise control of structural and interfacial interactions in hybrid systems. In this context, nanohybrids based on graphene oxide (GO) and polyaniline (PANI) have attracted considerable attention due to the combination of the high functionalization of GO with the conjugated structure and multiple oxidation states of PANI, resulting in materials with tunable properties. Interactions between the oxygen-containing functional groups of GO and the polymeric chains of PANI play a central role in modulating the physicochemical and thermal properties of hybrid

In this work, GO@PANI nanohybrids with different mass ratios (1:1, 1:4, and 3:4, GO:PANI) were synthesized and characterized with the aim of relating the composition to the interfacial interactions of the material. Fourier transform infrared spectroscopy (FTIR) revealed characteristic bands of the nanohybrid in all samples, with variations in intensity (Figure 1a) relative to the bands associated with the oxygenated groups of GO (O–H and C–O) and the N–H and C–N vibrations of PANI, indicating different degrees of interaction between the phases. A reduction in the GO fraction led to more pronounced interfacial interactions.

Raman spectroscopy confirmed the presence of H1 (~1350 cm^{-1}) and H2 (~1580 cm^{-1}) bands in all samples, with an increase in the H1/H2 intensity ratio, broadening, and small spectral shifts of the H1 band (Figure 1b) in the sample with the highest PANI content, indicating greater structural disorder associated with stronger GO–PANI interactions. Thermogravimetric analyses (TG/DTG) showed that the GO@PANI 1:4 hybrid exhibits greater thermal stability, indicating better structural integration between the phases. These results demonstrate that the GO/PANI mass ratio is a fundamental parameter in the development of GO@PANI nanohybrids with optimized structural and thermal properties.

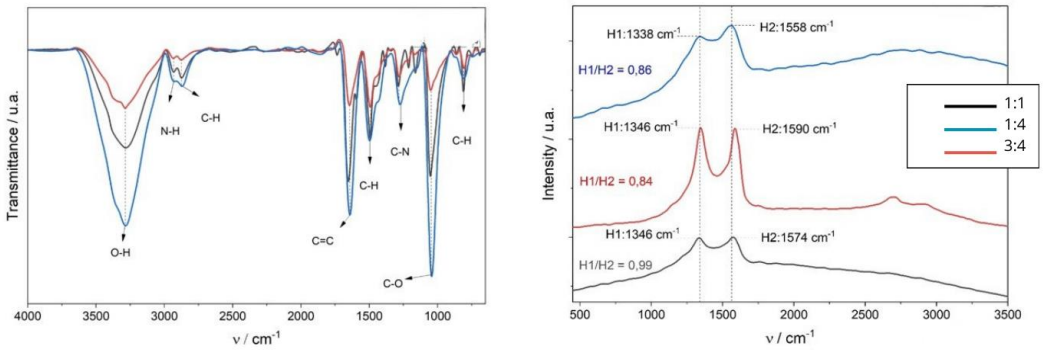


Figure 1: a) FTIR b) Raman Comparative spectra of GO@PANI, 1:1 Black, 3:4 Red and 1:4 Blue.

Agradecimentos/Acknowledgments

The authors thank CAPES for the master's scholarship at CEFETMG; Fapemig and CNPQ for support and the Characterization and Metrology Team of CTNANO/UFMG for the analyses.

Tuning optical properties of ZnGa2O4 nanoparticles with different dopants

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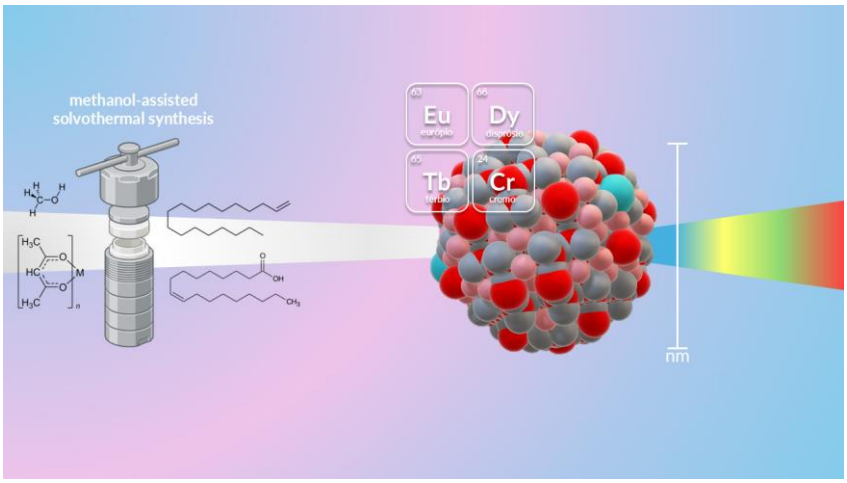
Palavras Chave:*synthesis,nanoparticles,luminescence,rare-earth*

Highlights

$ZnGa_2O_4$nanoparticles dopped with different elements. Synthesis via methanol-assisted solvothermal method. Crystalline and monodisperse system.

Resumo/Abstract

Zinc gallate ($ZnGa_2O_4$- ZGO) is a highly attractive crystalline host for engineering photonic sources via doping with different types of spectroscopically active ions. The combination of intrinsic and extrinsic defects causes local distortions responsible for the creation of traps in the electronic structure of this host, which is often associated with persistent luminescence phenomena. In the ZGO spinel structure, two cationic sites (Zn^{2+} and Ga^{3+}) can accommodate impurities such as trivalent lanthanides (Ln^{3+}), which preferentially replace Ga^{3+} in the octahedral sites leading to the rearrangement of electronic structure. In addition, transition metal ions such as Cr^{3+} have also been reported as responsible for producing near-infrared persistent luminescence. However, there is a still lack in the literature about X-ray sensitive persistent luminescence materials, which are highly relevant for medical applications. Based on the versatility of ZGO, we have chosen this host for the development of X-ray persistent scintillating materials and to achieve this goal, Ln^{3+} (Ln = Eu, Tb or Dy) and/or Cr^{3+} as dopants. ZGO and doped-ZGO have been synthesized using a methanol-assisted solvothermal as schematically depicted in Figure 1. Preliminary characterization has shown the formation of crystalline ZGO with broadened diffraction peaks, which suggest the formation of nanosized crystallites. No secondary crystalline phases were observed. Particle size distribution has been analyzed by dynamic light scattering (DLS) and ζ-potential and the results indicate promising and monodisperse system with average particle size in order of 10±5 nm. By photoluminescence, typical Ln^{3+} emission lines were observed, besides intrinsic defect-related broad emissions.



Solvothermal synthesis yields doped ZnGa2O4 nanoparticles with wavelength-tunable luminescence.

Agradecimentos/Acknowledgments

The authors thank FAPESP (24/20543-3, 22/03442-3 and 21/08111-2), CNPq and CAPES for the financial support. They are also grateful to the host institution for their facilities.

Tuning Plasmonic Response and Stability of Gold Nanorods through Surface Chemistry and Medium Conditions

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Palavras Chave:*Nanomedicine,Gold Nanorods,Experimental Design,Photothermal,Bio-Nanointerface*

Highlights

Protein adsorption and ionic strength are the main factors modulating AuNR physicochemical behavior.

PEGylation alters surface charge, LSPR position, and colloidal stability of gold nanorods.

Resumo/Abstract

Gold nanorods (AuNRs) are plasmonic nanostructures whose optical and colloidal properties are highly sensitive to surface chemistry and dispersion conditions. This study systematically investigates the effects of temperature, ionic strength, and protein adsorption on the physicochemical behavior of AuNRs stabilized with cetyltrimethylammonium bromide (CTAB) and modified with polyethylene glycol (PEG-SH). The replacement of CTAB by PEG was motivated by the intrinsic toxicity and limited colloidal stability of CTAB-based systems. A Rotational Central Composite Design (2^4) combined with Response Surface Methodology was employed to evaluate the influence of these factors on the polydispersity index (PdI), Zeta potential, and localized surface plasmon resonance (LSPR) wavelength, enabling the identification of significant effects and interactions with a reduced number of experiments. Protein adsorption and ionic strength emerged as the dominant parameters governing AuNR behavior. In CTAB-stabilized AuNRs, protein adsorption promoted Zeta potential inversion, while both protein adsorption and ionic strength significantly affected the LSPR wavelength ($p < 0.05$). PEGylated AuNRs exhibited enhanced colloidal stability and a more complex response profile, with significant quadratic and interaction effects involving protein adsorption, temperature, and ionic strength. Multivariate optimization identified an optimal condition at 15% protein concentration, balancing colloidal stability and optical response. These results underscore the importance of environmental factors in modulating AuNR surface properties, with direct implications for their plasmonic and photothermal performance.

Agradecimentos/Acknowledgments

Financial support from CAPES process number 88887.001902/2024-00 and CNPq projects 407961/2023-2 and 306413/2024-8.

Tuning the hierarchical pore structure of alumina supports via PEG molecular weight control

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Palavras Chave:*Alumina, hierarchical structures, porosity, PEG*

Highlights

Hierarchical γ-Al_2O_3 synthesized via PEG-mediated spinodal decomposition. Tuning PEG molecular weight to tailor pore sizes (6–28 nm) and specific superficial area (259 – 325 m^2/g)

Resumo/Abstract

Hierarchically structured inorganic porous materials have found applications in various fields, including energy storage, drug delivery, and catalysis, where the precise control over pore size is essential. Macropores serve as effective transport channels that facilitate a fast mass transfer. This structural feature might be particularly advantageous for the hydrotreatment of biomass, a key process in producing hydrotreated vegetable oil (HVO) as a renewable alternative to fossil fuels. In this work, hierarchical porous alumina was synthesized via sol-gel method to serve as a robust catalyst support. Porosity control was achieved through spinodal decomposition during the sol-gel transition, induced by the addition of polyethylene glycol (PEG) with molecular weights ranging from 200 to 8000 g/mol. Structural characterization using X-ray diffraction (XRD) confirmed the formation of γ-Al_2O_3 in all samples. Small-angle X-ray scattering (SAXS) data indicated a consistent radius of gyration of approximately 1.9 nm, suggesting the assembly of organized primary particles. Furthermore, a Porod exponent of approximately -4.0 across all samples indicated the presence of non-fractal objects with smooth surfaces. Nitrogen physisorption isotherms revealed that increasing the PEG molar weight from 200 to 8000 g/mol resulted in an increase in specific surface area from 259 to 325 m^2/g and an expansion of the average pore size from 6 to 28 nm. These findings demonstrate that this hierarchical alumina is a highly promising catalyst support for biomass hydroprocessing applications.

Agradecimentos/Acknowledgments

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Unveiling the modulation of SiO2 spheres by design of experiments (DoE)

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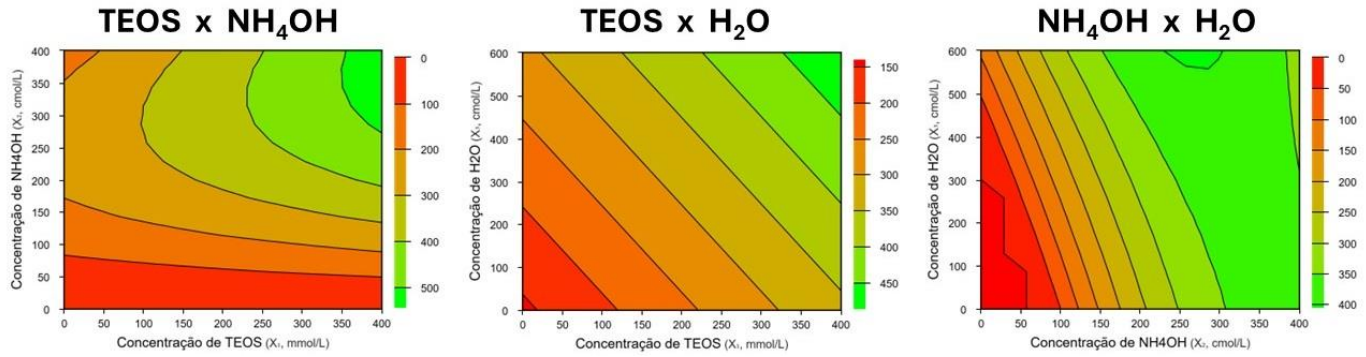
Palavras Chave:*Nanotechnology,silica,synthesis,Stöber method,RCCD*

Highlights

The experiment matrix generated spheres with diameters between 100-500 nm. Experimental data were well fitted by the adjusted models. Synthesis of 200 nm spheres were performed for validation.

Resumo/Abstract

In the field of nanotechnology, SiO_2 spheres appear as building blocks for a wide variety of applications. They can be used in heterogeneous catalysis, drug delivery systems, biomedical imaging, optoelectronics, coating and composites and energy storage (2024; TANJINDAPRATEEP, Adv. Matter. Sci. Res., 7, 191-192). The size of SiO_2 nanoparticles is often a key factor for many of those applications. Therefore, several studies can be found on the impact of different synthesis parameters on the spheres size. However, most of them are based on one-factor-at-a-time (OFAT) testing, which presents some disadvantages and limitations compared to design of experiments (DoE). In this study, DoE was employed on the synthesis of SiO_2 spheres by Stöber method. The reactants concentrations (TEOS, NH_4OH, H_2O) were evaluated by a three-variable DCCR matrix. The materials' morphologies and dimensions were confirmed by scanning electron microscopy (SEM) allowing mean size calculations and histograms. SEM data also confirmed that all materials were composed of SiO_2 spheres. The statistical evaluation of the DCCR matrix showed that the variables present first and second order effects on the particles' size. Among the latter, interaction effects were observed between TEOS and NH_4OH, and also between NH_4OH and H_2O. This is an important contribution of this work because interaction effects cannot be identified by OFAT. Mathematical models correlating the reactants concentrations with SiO_2 particle size and 4 other responses were obtained from DCCR data statistical treatment. Validation experiments focused on synthesizing spheres of 200 nm, and the experimental value (216 ± 14 nm) corroborated the model. Similar results were observed for the other responses. Therefore, DoE gave important insights into the reactants' effects on the synthesis of SiO_2 spheres. Moreover, it provided models which allowed a precise modulation of the particles' size.



Surface response of SiO2 particle size model obtained from DCCR matrix.

Agradecimentos/Acknowledgments

The authors thank CNPq and FAPERJ for financial support, LABNANO-CBPF and CENANO-INT/SISNANO (CNPq-SisNANO 442604/2019–0) for SEM analyses.

Unveiling the thermal decomposition kinetics of crystalline carbon nitrides: a study using the isoconversional method and artificial neural network

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Palavras Chave:*Poly(heptazine) imide,mechanistic kinetic models,thermal treatment,porosity*

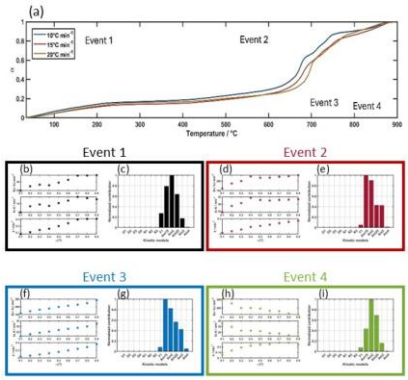
Highlights

The thermal decomposition of crystalline carbon nitrides follows nucleation kinetic mechanisms models, indicating changes in structure that influence their catalytic and adsorption activities.

Resumo/Abstract

Carbon nitrides (CN) are promising catalytic materials, though they often suffer from limited surface area and porosity. Due to their structural similarity to graphene—both consisting of stacked 2D layers—rapid heat treatments could enhance specific surface area via explosive exfoliation driven by released gases [1,2]. Literature reports confirm that thermal treatment of graphitic carbon nitride (g-C_3N_4) increases its porosity and photocatalytic efficiency for hydrogen evolution [2]. However, are the thermal decomposition mechanisms and kinetics analogous to those of graphene oxide (GO), where gas diffusion governs the initial step, followed by a nucleation mechanism that generates defects and holes? Given the significantly higher thermal stability of CNs compared to GOs, the mechanism likely differs. Previously, the authors studied GO thermal decomposition kinetics via an isoconversional method using artificial neural networks applied to thermogravimetric (TG) data [3]. Here, this approach is applied to a crystalline CN, specifically poly(heptazine imide) (PHI). The results reveal a more complex process involving four distinct decomposition events. The kinetics for all events follow Avrami-Erofeev nucleation models, describing the formation of nuclei with varying crystallinity and chemical structure that grow and propagate through the material during decomposition. Pristine and heat-treated PHI samples will be comprehensively characterised by XRD, FTIR, XPS, solid-state NMR, TEM, and N_2 adsorption.*In-situ*monitoring will track structural evolution during thermal treatment. Additionally, TG coupled with MS and/or FTIR will identify evolved gases. This integrated methodology aims to predict the porous structure of thermally modified CNs, enabling their optimised use in catalysis and adsorption applications.

References: [1] Chem. Phys. Lett. 807 (2022), 140091. [2] Appl. Catal. B-Environ. 233 (2018), 80-87. [3] Thermochimica Acta 721 (2023), 179454.



(a) Conversion degree curves; (b,d,f,h) Kinetic parameters; (c,e,g,i) normalized contribution model.

Agradecimentos/Acknowledgments

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Urban Mining and Circular Economy in the Synthesis of Ceramic Materials

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Palavras Chave:*Urban mining,Electronic waste,Rare earths,Magnets,Ceramic materials*

Highlights

Urban mining applied to magnets from electronic waste;
Acid leaching to obtain a rare-earth-rich solution;
Direct use of the leachate in the sustainable synthesis of ceramic materials.

Resumo/Abstract

The increasing disposal of electronic waste has intensified the need for sustainable strategies to recover high-value metals, particularly rare earth elements present in permanent magnets. The dependence on primary sources and the environmental impacts associated with conventional mining reinforce the demand for approaches based on the circular economy. In this context, urban mining stands out as a promising alternative for valorizing such residues, enabling the reinsertion of strategic metals into new production chains. This study aims to utilize metals recovered from discarded hard disk drive (HDD) magnets for the sustainable synthesis of ceramic materials, directly employing the leachate obtained from the hydrometallurgical step as a precursor. Previously ground and demagnetized magnets were subjected to acid leaching with sulfuric acid, as described in the scheme shown in Figure 1. The chemical composition of the leachate was determined by inductively coupled plasma optical emission spectrometry (ICP-OES), revealing a multielement solution rich in neodymium, praseodymium, and other metals from the magnet matrix. The leachate was directly used in the synthesis of a ceramic material, which was subsequently characterized by X-ray diffraction to identify the crystalline phases formed. The results demonstrated that the direct use of the leachate as a ceramic precursor represents a technologically viable and environmentally sustainable approach, as it reduces the need for additional purification steps, minimizes reagent and energy consumption, and promotes the valorization of electronic waste through its conversion into higher value-added materials.

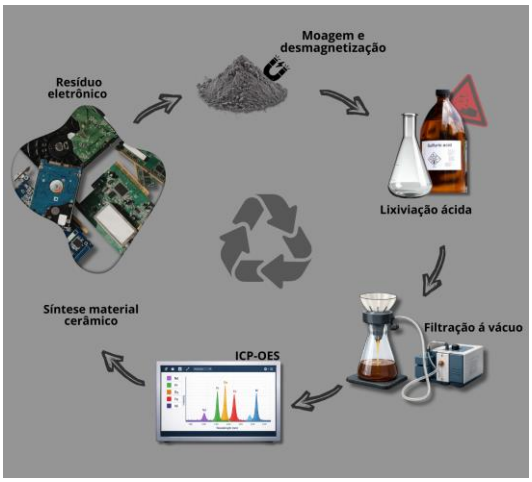


Figure 1: Methodological process for the synthesis and analysis of the leachate

Agradecimentos/Acknowledgments

UFOP; PPGQUIM; CAPES; CNPq; FAPEMIG

Use of dolomite limestone in neutralization of vinasse to biofertilizerproduction

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Palavras Chave:*Vinasse, dolomite limestone, biofertilizer.*

Highlights

Vinasse generation is a challenge in the sugar-ethanol industry. Potentiometric titration defined limestone mass for neutralization. Dolomitic limestone addition enriched vinasse with Ca and Mg.

Resumo/Abstract

The agro-industrial sector faces the challenge of balancing economic performance with environmental sustainability, making effective waste management a key concern. In this context, the sugar and alcohol industries generate large volumes of vinasse, a byproduct of ethanol production, at an average ratio of approximately 15 L of vinasse per liter of ethanol. Despite its environmental impact, vinasse presents significant potential as a biofertilizer due to its high levels of macro- and micronutrients. Nevertheless, its acidic nature and elevated levels of chemical and biochemical oxygen demand limit direct application and promote rapid degradation. This work aimed to evaluate the use of commercial dolomitic limestone as a neutralizing agent for the preliminary treatment of vinasse. The alkalinity of the limestone and its capacity to enrich the medium with calcium (Ca) and magnesium (Mg), essential macronutrients for soil fertility, were investigated. Potentiometric titration was used to determine the mass of dolomitic limestone required for vinasse neutralization. The results (Figure 1) showed that 0.55 g of dolomitic limestone was required for 100 mL of vinasse, effectively correcting acidity while simultaneously increasing Ca and Mg availability. These findings highlight the potential of chemically treated vinasse as a value-added agricultural input. Further studies will explore processing strategies to enhance stability and facilitate practical application.

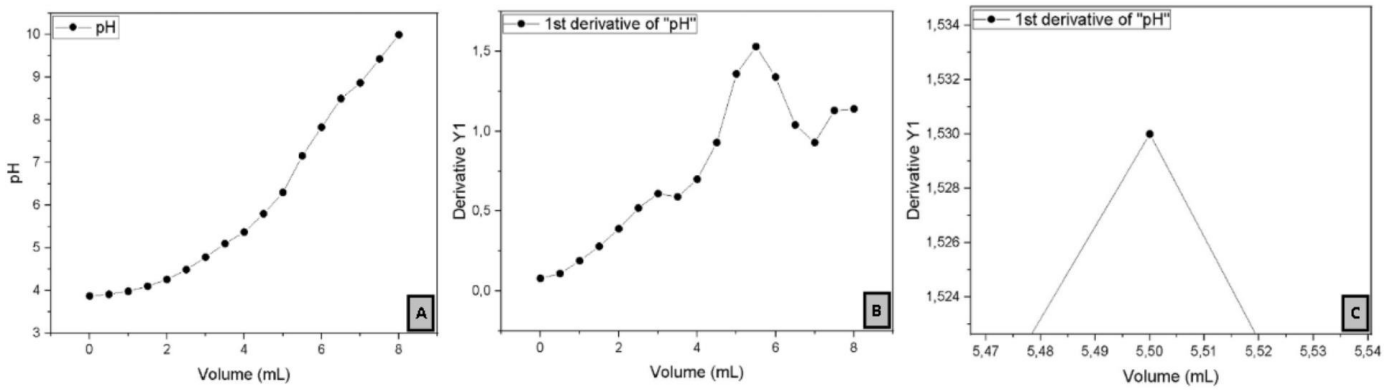


Figure 1: Titration curve (a); derivative (b); approximate equivalence point (c). Source: Author.

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CNPq, INEO and FAPESP

Use of mixed nitrogen precursors for N-doped activated carbon with Alpaca fiber: Optimization by Simplex-Centroid Design

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Palavras Chave:*): N-Doped Activated Carbon, Simplex-Centroid Design, Alpaca Fiber,N-Doped Activated Carbon,Simplex-Centroid Design,Alpaca Fiber*

Highlights

Use of alpaca fiber to produce activated carbon

Use of 3 nitrogen precursors as a misture for N-dopped activated carbon

Simplex-centroid design utilization for optimization of nitrogen precursor ratio

Resumo/Abstract

Activated carbon (AC) is widely used in various applications, including contaminant adsorption and clean energy production. Doping with heteroatoms, such as nitrogen, can enhance properties like electrical conductivity, affinity for polar species, and the creation of new active sites for catalytic and adsorption processes. The production of nitrogen-doped activated carbon (NAC) has attracted significant interest in the field of materials science; however, the use of multiple nitrogen sources and the evaluation of their synergy for doping in AC remain underexplored areas.

This study aims to investigate the preparation of nitrogen-doped activated carbon optimized through the simplex-centroid statistical tool. Alpaca fibers, widely used in the textile industry in South America, generate approximately 4 million tons of waste annually, making them a promising precursor for AC production. Activated carbon was prepared using KOH and varying proportions of nitrogen sources such as melamine, urea, and hexamethylenetetramine (HMTA), with the objective of optimizing a nitrogen-doped material. The optimization was carried out using the BET surface area (SBET) and nitrogen percentage (%N) as responses.

The results indicated that SBET ranged from 181 to 1851 $m^2\ g^{-1}$, while %N varied from 3.43% to 10.15%. After applying the simplex-centroid design, it was observed that the experimental data violated the assumptions of normality and homoscedasticity of the residuals, requiring data transformations. For SBET, the cubic model, and for %N, the linear model were found to be the most significant, according to ANOVA. The optimal precursor proportions were 0.403 g of melamine, 1.0230 g of HMTA, and 1.5730 g of urea, resulting in a SBET of 1304 $m^2\ g^{-1}$ and a %N of 4.66%. The experimental values obtained with these proportions were 1631 $m^2\ g^{-1}$ and 4,15%, with variation between the theoretical and experimental values of 20 and 10,9%, respectively.

Agradecimentos/Acknowledgments

CAPES, COMCAP, CNPQ, DQI/UEM, GMCM

Valorização de rejeito de mineração de ferro para obtenção de sílica mesoporosa aplicada à captura de CO2

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Palavras Chave:*Sílica mesoporosa,Rejeito de mineração de ferro,Captura de CO2,Economia circular*

Highlights

Iron ore tailings were used as an alternative Si source. Ordered mesoporous silica with high surface area was obtained. The material was efficient for CO_2 capture.

Resumo/Abstract

A sílica mesoporosa é um adsorvente promissor para captura de CO_2 devido à sua elevada área superficial específica e estrutura de poros ordenados. Nesse contexto, rejeitos do beneficiamento de minério de ferro, ricos em SiO_2, representam uma matéria-prima alternativa de baixo custo para a produção desse material, além de contribuir para a valorização de resíduos da mineração. Assim, este trabalho teve como objetivo sintetizar sílica mesoporosa a partir de rejeito de mineração de ferro e avaliar sua aplicação na captura de CO_2. O rejeito, coletado na mina de Brucutu (Vale), foi lixiviado com HCl para remoção de metais e submetido a tratamento hidrotérmico com NaOH (200 ºC) para obtenção de silicato de sódio, utilizado em substituição ao tetraetilortossilicato (TEOS). A estrutura mesoporosa foi direcionada pelo surfactante CTAB e, após calcinação a 540 ºC, obteve-se o material poroso. A caracterização do rejeito indicou SiO_2(68,97%) e Fe_2O_3 (25,45%), além de morfologia heterogênea e tamanho médio de partículas de 111,5 ± 65,9 µm. A sílica apresentou área superficial específica de 1012 $m^2\ g^{-1}$, volume de poros de 0,61 $cm^3\ g^{-1}$ e diâmetro médio de 3,81 nm, confirmando sua mesoporosidade e potencial para captura de CO_2. A microscopia eletrônica de varredura (MEV) e a espectroscopia de energia dispersiva (EDS) indicaram partículas aproximadamente esféricas em escala nanométrica, com predomínio de Si e O e distribuição homogênea desses elementos. A microscopia eletrônica de transmissão (Fig. 1) corroborou esses resultados, evidenciando partículas em torno de 160 nm e um alto grau de ordenamento dos mesoporos. A captura de CO_2 foi avaliada a 273, 283 e 298 K, obtendo-se 1,53, 1,25 e 0,88 mmol g^{-1}, respectivamente, a 1 bar. O aumento da temperatura reduziu a adsorção, consistente com o caráter exotérmico do processo. Os resultados demonstram a viabilidade de converter rejeitos da mineração em adsorventes para mitigação de CO_2.

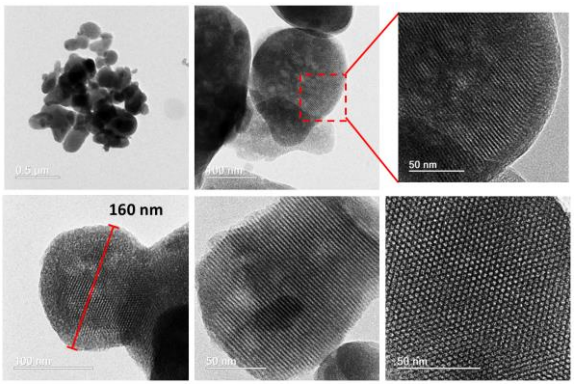


Fig 1. Microscopia eletrônica de transmissão da sílica obtida a partir do rejeito de ferro.

Agradecimentos/Acknowledgments

Os autores agradecem à UFMG, à FAPEMIG e à CAPES pelo apoio financeiro, ao Grupo de Tecnologias Ambientais (GRUTAM) pela infraestrutura e ao Laboratório Nacional de Nanotecnologia para o Agronegócio (LNNA) pelo auxílio nas análises.

VALORIZAÇÃO DOS RESÍDUOS DA COROA DO ABACAXI (Anans comosus) VIA PIRÓLISE PARA A OBTENÇÃO DE INSUMOS DE INTERESSE INDUSTRIAL

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Palavras Chave:*Biomassa lignocelulósica,Pirólise,Coroa do abacaxi,Bioenergia*

Highlights

A pirólise da coroa do abacaxi gerou BTEX e compostos oxigenados a partir de biomassa lignocelulósica rica em hemicelulose e celulose, evidenciando potencial para bioenergia e insumos químicos.

Resumo/Abstract

A crescente demanda energética ocasionou a busca por fontes sustentáveis de energia e a diversificação da matriz energética[1]. Diante disso, as biomassas lignocelulósicas destacam-se pelo potencial bioenergético, tornando os resíduos da indústria agrícola uma possível fonte de matéria prima para produção de insumos químicos[2]. Neste sentido, a pirólise desses materiais torna-se uma alternativa viável, devido à sua versatilidade e condições mais brandas de conversão[3]. O presente trabalho teve como objetivo a pirólise da coroa do abacaxi, para obter substâncias de interesse industrial. Os resíduos da coroa de abacaxi foram adquiridos de empresas localizadas na microrregião de Itapetinga/BA. As coroas foram lavadas para remoção de impurezas, secas em estufa e posteriormente trituradas. Em seguida foram caracterizadas quanto ao teor dos biopolímeros, umidade e cinzas. Posteriormente foram submetidas à pirólise em um equipamento EGA Py 3030D (Frontier) acoplado a um espectrômetro de massas (Shimadzu). As análises foram feitas em duplicata e as substâncias identificadas por tentativa utilizando o webbook da National Institute of Standards and Technology (NIST). As análises da pirólise da coroa do abacaxi indicaram um teor de umidade e teor de cinzas igual a 8,63% e 4,49% respectivamente. Observou-se ainda um elevado conteúdo de hemicelulose (35,64%) e celulose (20,96%), aliado a um baixo teor de lignina (2,66%). A pirólise térmica do material revelou a presença de alguns BTEX (benzeno, tolueno, etilbenzeno e xilenos). Dentre os BTEX identificados, o tolueno apresentou maior teor relativo (4,65%), foi identificado um baixo percentual de xilenos (1,28%) e elevado teor de compostos oxigenados, como 4-vinil-fenol (26,20%), furfural (11,39%), 5-Hidroximetilfurfural (2,58%) e fenol (8,69%). Neste sentido, os resultados obtidos sugerem potencial da coroa do abacaxi como matéria prima para pirólise visando a obtenção de substâncias com valor alto agregado.

Agradecimentos/Acknowledgments

Os autores agradecem à Fundação de Amparo à Pesquisa do Estado da Bahia pela bolsa concedida e à Universidade Estadual do Sudoesta de Bahia (UESB) e à Universidade Federal do Rio Grande do Sul pela infraestrutura concedida.

Vidros borofosfato como aditivos antimicrobianos para membranas poliméricas eletrofiadas

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Palavras Chave:*Vidro,Borofosfato,Eletrofiação,Polímero*

Highlights

Electrospun PVA and Ecovio® membranes with borophosphate glass showed antimicrobial activity against*S. aureus*and*E. coli*, with superior performance for PVA-based systems.

Resumo/Abstract

As superbactérias são micro-organismos resistentes, cujo surgimento está associado ao uso inadequado de antibióticos, representando um desafio crescente para a saúde pública. Nesse contexto, o desenvolvimento de materiais com atividade antimicrobiana torna-se fundamental, especialmente para aplicações em curativos e engenharia de tecidos. Os polímeros são materiais estudados na engenharia de tecidos e podem contribuir para a reestruturação da pele. Nesse estudo membranas poliméricas eletrofiadas à base de PVA e Ecovio® foram incoporadas com um vidro borofosfato livre de metais de transição e com atividade antimicrobiana. O vidro foi obtido pelo método de fusão-resfriamento a partir de KH_2PO_4, $NH_4H_2PO_4$ e H_3BO_3, a 400 °C por 1 hora. As membranas poliméricas foram obtidas pelo processo de eletrofiação. Para o polímero PVA (Álcool-polivinílico, grau de hidrolize 99%) foi preparada uma solução com a concentração de 8%(m/v) do polímero, 85% de água (v/v), 15% (v/v) de uma solução de vidro borofosfato, e 5%(m/v) de ácido cítrico (agente reticulante). Procedeu-se a eletrofiação com uma tensão de 10 kV, vazão de 1,0 mL/h e coletor rotativo a 600 rpm.Após a eletrofiação, a membrana foi reticulada em estufa a 180°C no período de 10 minutos. Para o polímero Ecovio® a solução foi prepadada com a concentração de 20%(m/v), 85% (v/v) de clorofórmio e 15% (v/v) de dimetilformamida. A eletrofiação foi realizada com um fluxo de 2 mL/h, tensão de 8 kV e coletor rotativo a 600 rpm. Para o Ecovio, o vidro foi inserido por meio de adsorção de uma solução concentrada. Foram realizados testes antimicrobianos frente as bactérias de*Stapylococcus aureus*e*Escherichia coli*, foi constatado que as membranas apresentaram atividade antimicrobiana frente as bactérias testadas.

Dessa forma, os materiais desenvolvidos mostram potencial para aplicação como curativos antimicrobianos, contribuindo para o combate a infecções bacterianas.

Agradecimentos/Acknowledgments

Agradecimentos a Universidade Estadual do Oeste do Paraná, a Universidade Tecnólogica Federal do Paraná, a Universidade Federal do Paraná e ao Conselho Nacional de Desenvolvimento Científico e Tecnológico.

49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

MED - Química Medicinal

Accelerated Antiparasitic Hit Discovery via Greener and Cost-Effective Microscale Parallel Synthesis of Heterocycles

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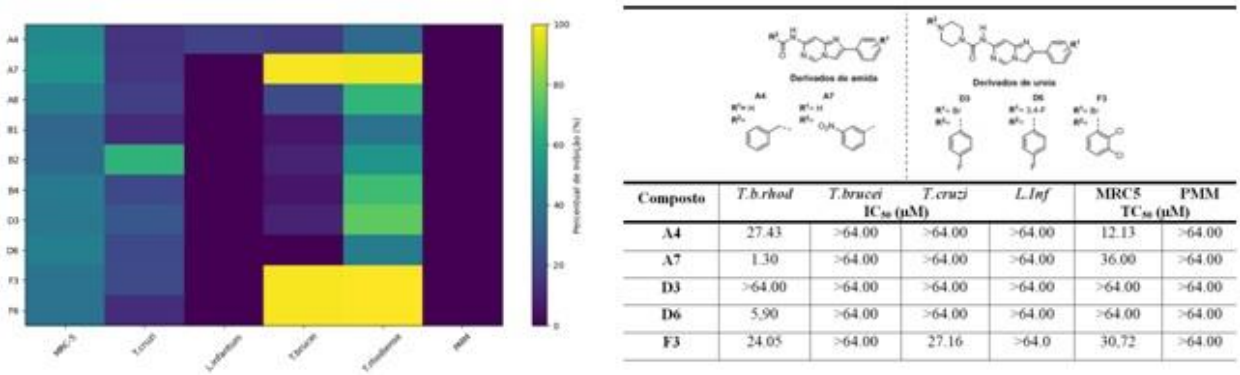
Palavras Chave:*Imidazopyrimidines, Antiparasitic drug discovery, Microscale parallel synthesis, Phenotypic screening, Structure–activity relationships*

Highlights

Greener microscale heterocycle synthesis enables rapid antiparasitic hit prioritization. Direct crude screening validates activity, while resynthesis confirms true hits and excludes artifacts.

Resumo/Abstract

Neglected tropical diseases require accelerated and resource-efficient medicinal chemistry strategies. Here we report a greener Microscale Parallel Synthesis **combined with Medium-Throughput Screening**(MPS–MTS) platform applied to the discovery of antiparasitic agents based on the imidazopyrimidine scaffold. A library of 96 imidazopyrimidine-derived ureas and amides (S1–S95) was generated using reduced reagent and solvent quantities, enabling sustainable chemical space exploration. Reaction mixtures were rapidly characterized by LC–MS and semi-quantitative ^{1}H NMR to confirm product formation and ensure equimolar normalization prior to direct phenotypic screening of crude mixtures. Compounds were evaluated at 64 µM against*Trypanosoma cruzi*,*Trypanosoma brucei*,*T. b. rhodesiense*, and*Leishmania infantum*, alongside cytotoxicity assessment in MRC-5 and PMM cells. Heatmap-guided analysis enabled rapid identification of distinct biological response profiles. T. brucei and T. b. rhodesiense were the most sensitive species. Mixtures corresponding to compounds A7, F3 and F6 showed >98% inhibition against both parasites. Ten representative mixtures were resynthesized and purified to validate activity and calculate IC_{50} values. Compound A7 emerged as the most potent analogue (IC_{50} = 1.30 µM against T. b. rhodesiense; SI > 27), confirming the predictive value of the crude screening strategy. In contrast, discrepancies observed for selected analogues revealed that residual triphosgene or reactive byproducts may generate false-positive cytotoxicity signals in crude samples. Overall, the MPS–MTS workflow reliably anticipates structure–activity trends, distinguishes true antiparasitic hits from artifacts, and significantly shortens the design–make–test cycle. This sustainable and cost-effective platform represents a promising strategy for accelerating antiparasitic drug discovery.



Composto	*T.b.rhod*	*T.brucei*	*T.cruzi*	*L.Inf*	MRC5	PMM
	IC_{50} (µM)				TC_{50} (µM)	
A4	27.43	>64.00	>64.00	>64.00	12.13	>64.00
A7	1.30	>64.00	>64.00	>64.00	36.00	>64.00
D3	>64.00	>64.00	>64.00	>64.00	>64.00	>64.00
D6	5.90	>64.00	>64.00	>64.00	>64.00	>64.00
F3	24.05	>64.00	27.16	>64.0	30.72	>64.00

Biological activity heatmap of MPS–MTS-synthesized compounds and their antiparasitic effects

Agradecimentos/Acknowledgments

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Affinity Selection Mass Spectrometry as a Platform for Identifying Cholinesterase Ligands from Natural Products

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Palavras Chave:*Alzheimer's disease,, Annona coriacea,Annona coriacea,Multitarget,Immobilization,Magnetic particles*

Highlights

Dual AChE/BChE modulation is a promising strategy to reduce symptoms in different stages of Alzheimer's disease. AS-MS revealed seven dual AChE/BChE ligands from*Annona coriacea*flower extract.

Resumo/Abstract

Alzheimer's disease (AD) leads to progressive cognitive impairment, in part due to dysregulation of the cholinergic system composed of acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). While AChE activity predominates in the early stages of AD, BChE becomes increasingly relevant as the disease progresses, reinforcing cholinesterases as complementary therapeutic targets.[1] In this context, the discovery of dual-target ligands capable of modulating AChE and BChE has emerged as a promising strategy. Notably, natural libraries are valuable sources of structurally diverse multitarget candidates, as evidenced by two drugs approved for clinical trials that are derived from natural products.[2] Herein, the flower extract of*Annona coriacea*was investigated as a potential source of dual-target ligands using affinity selection mass spectrometry (AS-MS). Both enzymes were immobilized onto commercial magnetic particles and incubated with the extract (3 mg/mL) at room temperature under gentle stirring for 30 min, in separate experiments. After magnetic separation, the supernatant S0 was collected and the immobilized enzymes were washed twice with ammonium acetate buffer (S1 and S2), followed by ligand elution with two conditions: methanol and heated methanol at 80 °C (S3 and S4). Control assays using inactivated AChE and BChE were performed to probe nonspecific interactions. Affinity ratios (AR) were calculated by comparing ligand peak areas from assays with active and inactive enzymes, and only compounds with AR ≥ 1.20 were considered ligands. LC–HRMS analysis of the supernatants indicated seven potential dual-target ligands with AR values ranging from 1.24 to 11.55 (Table 1). Structural annotation of the identified ligands is currently underway. Overall, AS-MS enabled screening of complex natural libraries, identifying promising dual-target candidates.

References:

[1]Pang, X. et al. Eur. J. Med. Chem. 2025, 289, 117453.

[2]Oliveira, P.C.O. et al. PRENAP 2024, 5, 100099.

Ligands #		1	2	3	4	5	6	7
RT (min)		10.47	11.77	14.06	15.21	15.26	15.27	15.46
m/z		321.1307	474.2333	463.2831	649.2831	686.4356	669.4461	706.4162
Ion mode		+	-	-	-	-	-	-
Affinity Ratio (AR)	AChE	1.70	5.12	1.29	1.40	1.30	1.37	1.61
	BChE	1.40	11.55	1.30	1.32	1.34	1.23	2.69
Fragments		167.0198 220.9155 143.9948 237.8717 199.0735	411.2400 275.1686 321.8941 44.9997 322.8765	281.2497 463.2813 282.2527 464.2835 279.2314	311.1663 45.0001 312.1711 325.1873 339.2025	325.1810 339.2004 326.1830 311.1647 340.2023	45.0010 325.1807 311.1678 339.1937 333.9358	311.1660 297.1541 325.1830 367.9206 279.2324

Table 1: LC-HRMS/MS analysis of the identified ligands.

Agradecimentos/Acknowledgments

CNPq, FAPERJ (E-26/202.111/2025 and E-26/210.547/2025), and CAPES – Finance Code 001.

Avaliação do potencial antifúngico da attinimicina

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Palavras Chave:*Sideróforo,Antifúngico.*

Highlights

Em meio à crescente emergência das micoses sistêmicas no cenário mundial e o aumento da resistência aos antifúngicos disponíveis, a attinimicina surge como uma proposta terapêutica inovadora.

Resumo/Abstract

A emergência das micoses sistêmicas é uma grave questão de saúde mundial, sendo os grupos marginalizados os mais afetados, como os imunossuprimidos (Bongomin et al., 2017). Os fármacos existentes apresentam problemas relacionados à resistência, reforçando a necessidade de fármacos com mecanismos de ação inovadores. O objetivo deste estudo foi avaliar o potencial antifúngico da attinimicina analisando seu possível mecanismo de ação, conformação e suas propriedades farmacocinéticas in silico. Pesquisas anteriores mostraram que a attinimicina tem atividade antifúngica significativa e pode atuar como sideróforo (Fukuda, et al. 2021), um comportamento promissor frente à resistência antimicrobiana (Ribeiro M, et al. 2021). Com isso, foi feita revisão bibliográfica com 7 artigos dos últimos 10 anos acerca da attinimicina, mecanismos de ação de sideróforos e seu potencial terapêutico.

A attinimicina apresenta uma média potência de complexação com Fe^{3+}, e portanto, o captura, de modo a torná-lo indisponível aos fungos do meio. Deste modo, sua atividade antifúngica está possivelmente relacionada com a privação de ferro daqueles que não possuem receptores de internalização desse sideróforo (Figura 1). Em paralelo, foi realizada a avaliação in silico da conformação, características físico-químicas e farmacocinéticas da attinimicina por meio da plataforma ADMET Lab 3.0 e outros softwares. Nas análises farmacocinéticas in silico, foi possível prever que tal molécula pode apresentar problemas de absorção e distribuição nos tecidos humanos, o que está relacionado com sua capacidade de se ionizar em pH fisiológico e diversidade de interações intermoleculares com proteínas plasmáticas. Com este estudo, foi possível ampliar o conhecimento sobre esse produto natural ainda pouco explorado, identificar suas limitações para aplicação antifúngica e obter embasamento científico para propor modificações estruturais para superar os pontos críticos e potencializar suas propriedades.

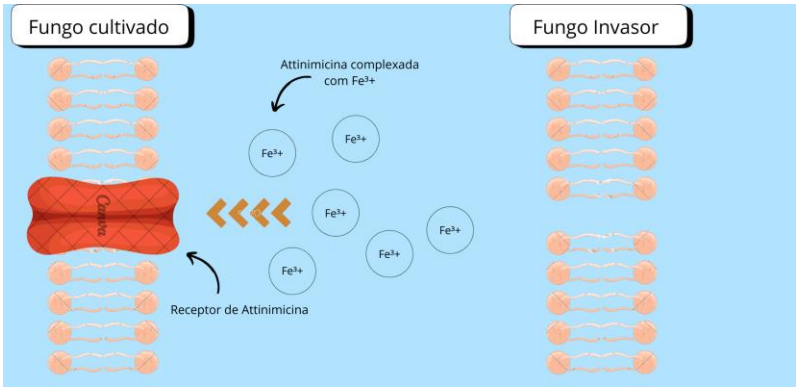


Ilustração do mecanismo de ação proposto. Imagem autoral.

Agradecimentos/Acknowledgments

V.F.M grato à Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) #2025/22748-4 e #2025/08250-3

BODIPYs as Fluorogenic Probes for Live-Cell Imaging of Lipid Droplets

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Palavras Chave:*BODIPY,C. elegans,lipid doplets*

Highlights

In this work, BODIPYs were identified as fluorogenic probes for live-cell imaging studies and Caenorhabditis elegans, being efficient and selective for lipid droplets.

Resumo/Abstract

The lipophilic fluorescent markers normally are a tool suitable to a wide range of biological applications such as optical sensor, qualitative and quantitative lipids evaluation, diagnosis components and lipids intracellular dynamics.[1] In this work, BODIPY-p-SMe was identified as fluorogenic probes for live-cell imaging studies and Caenorhabditis elegans, being efficient and selective for lipid droplets. The compound BODIPY-p-SMe stained cellular lipid droplets in all tested samples (Figure 1), showing impressive results, binding to a large number of lipid bodies and producing high-intensity green fluorescence emission.*Caenorhabditis elegans*(*C. elegans*) are non-pathogenic nematodes extensively used as a model organism to investigate many cellular mechanisms in more complex mammalian organisms. This nematode is widely used to assess lipid synthesis and dynamics.[2] Our results demonstrated outstanding staining of lipids inside the cells distributed for all nematode body mainly lining the*C. elegans*gut (Figure 1C). When the staining pattern produced by compound BODIPY-p-SMe was compared with those produced by Oil red® and Nile Red®, that are two lipid bodies commercially available and widely used in the literature, we observed a better stain and less background staining in the samples with BODIPY-p-SMe (Figure 1C-E). Finally, we have demonstrated here that the compound BODIPY-p-SMe synthetized and tested by us have lipid affinity and can be proposed as a novel lipid droplet dye which can be used to stain lipids inside isolated mammal cells or in complex tissues as has been shown in this work through*C. elegans*lipid staining.

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[2] Witting, M.; Schmitt-Kopplin, P.*Arch. Biochem. Biophys.*,**2016**,*589*, 27.

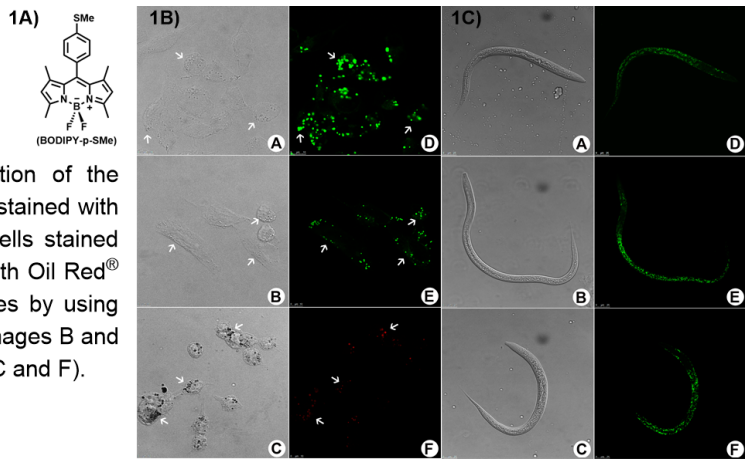


Figure 1. 1A) Chemical structure of the compound BODIPY-p-SMe **1B)** HUVEC cells co-staining assay with the compound BODIPY-p-SMe, Oil red® or Nile Red® in fixed samples. Images A, B and C show the normal cells morphology by phase contrast microscopy after incubation of the samples with each tested compound. Image D shows cells stained with the compound BODIPY-p-SMe (green), image E shows cells stained with Nile Red® (green) and image F shows cells stained with Oil Red® (red). **1C)** Co-staining assay with *C. Elegans* fixed samples by using Nile Red® (images A and D), compound BODIPY-p-SMe (images B and E) and compound BODIPY-p-SMe plus Nile Red® (images C and F).

Figure 1

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPERJ, UNB, UFF.

Chiral Selectivity of Mn3O4 Nanoparticles Functionalized with Mannonic Acid in Ovalbumin and CD14 binding: Implications for Anti-Tumor Immune Response

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Palavras Chave:*Chiral Mannonate–Trimanganese Tetroxide Nanoparticle,Ovalbumin,Cluster of differentiation 14 (CD14),Molecular Dynamics Simulation*

Highlights

Chiral mannonate–Mn_3O_4 NPs were designed.

D- and L-NPs bind differently to ovalbumin and CD14.

L-NP interaction were stronger and more persistent.

Target-proteins were enantioselectives for L-NPs.

Resumo/Abstract

Here, we modeled a nanoparticle with chiral trimanganese tetroxide (Mn_3O_4) core functionalized with chiral mannonic acid ligands for potential application in cancer management. Spheroidal nanoparticles were modeled with a diameter of 2.4 nm and a stoichiometry $Mn(II)_{68}Mn(III)_{179}O_{336}^{+}$. Geometry optimization was carried out on semiempirical density functional theory (DFT) using the extended tight-binding (xTB) method with the GFN1-xTB Hamiltonian. The nanoparticle surface was, then, saturated with 32 mannonate ligands, resulting in a composition of $[Mn(II)_{68}Mn(III)_{179}O_{336}(\text{D-mannonate})_{32}]^{31-}$ and submitted to an additional xtb optimization step. The optimized nanoparticle (D-NP) and its mirror image (L-NP) were simulated using CHARMM36 force field in GROMACS 2025.1. Four systems were constructed: (1 and 2) four D-NPs placed around either the ovalbumin (OVA) or the cluster of differentiation 14 (CD14) structures; and (3 and 4) the corresponding protein systems with four L-NPs placed around them. The MD protocol included: (a) energy minimization to remove repulsive contacts; (b) NVT equilibration step with temperaure increasing from 0 K to 309.65 K and integration timestep adjusted from 0.5 to 1 fs under position restraints of proteins and NPs; (c) NVT step with no restraint at 309.65 K and Δt = 1 fs; (d) NpT equilibration (200 ns, 309.65 K, Δt = 1 fs, 1 bar under Berendsen barostat); (e) NpT production step (800 ns, 309.65 K, Δt = 1 fs, and 1 bar under Parrinello-Rahman barostat). L- and D-NPs exhibited distinct interaction patterns with the target proteins. In the OVA system, L-NPs showed stable and long-lived binding, whereas D-NPs displayed no sustained interaction. For CD14, L-NPs interacted with multiple domains, while D-NPs presented a delayed and weaker binding limited to a terminal region. Overall, the results indicate a clear enantioselective preference for L-NPs, consistent with experimental evidence in cancer-related experiments.

Agradecimentos/Acknowledgments

We acknowledge FAPESP (Center for Molecular Engineering for Advanced Materials – CEMol/CEPID process 2024/00989-7) and CNPq (311352/2022-7) support and the HPC resources from the SDumont supercomputer.

CODETAC: COmputer-Driven platform to Explore new TArgets and design small molecules and Chimeras from Brazilian biodiversity and experimental data

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Palavras Chave:*drug discovery,high throughput screening,natural products,crystallography,molecular modeling*

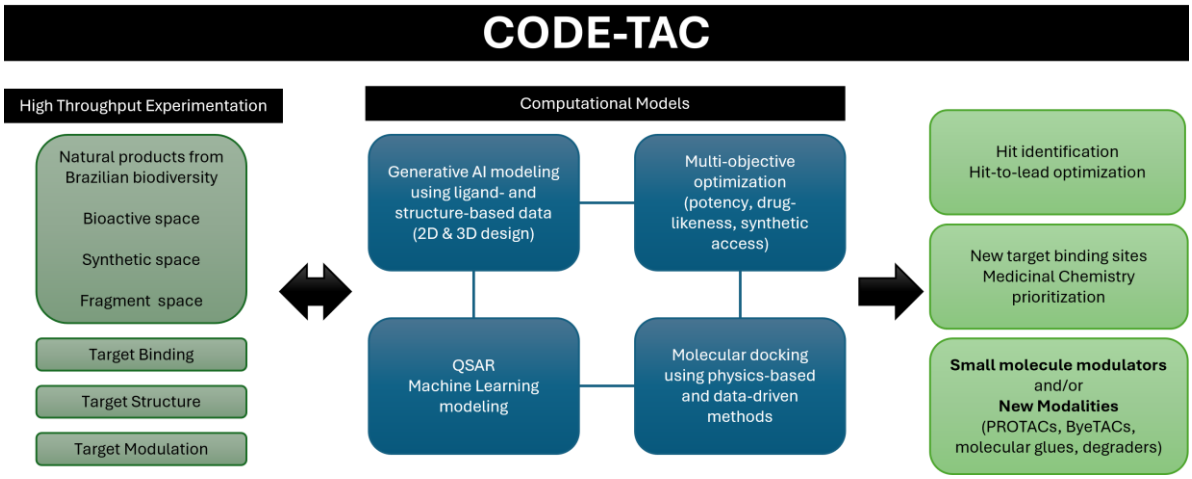
Highlights

Platform integrating generative AI, multi-objective optimization, high-throughput experimental screening & biodiversity

Prioritization & discovery of new target binding sites, modulators and degraders

Resumo/Abstract

The discovery of bioactive molecules for complex biological targets remains a challenge, particularly for diseases that are poorly addressed by conventional drug discovery workflows. Here, we present a platform that combines experimental screening, Brazilian biodiversity, and AI generative modeling to accelerate hit discovery and optimization. Our workflow begins with the acquisition of biological structural data from fragments and natural products screening and/or biochemical/binding assays data from high-throughput methods. This allows assessing large compound libraries with key chemical-biological experimental information. Fragments and natural products on crystallographic screening campaigns serve as probes, revealing novel target binding sites. Whereas HTS data serves as training sets for developing QSAR machine learning models. Protein-ligand complexes as well as predictive QSAR models are thus used to constrain 2D/3D generative AI models, guiding the exploration of biologically relevant chemical space. Generated compounds are subsequently evaluated by consensus and ensemble docking using physics- and data-driven approaches. These steps are accompanied by multi-objective optimization, accounting for potency, drug-likeness, synthetic accessibility and structural novelty. Beyond small-molecule drug discovery, the platform enables the exploration of new drug modalities, such as PROTACs, ByeTACs, and molecular glues, by favoring the identification of ligands able to bind on exposed and previously unexplored sites on target proteins. By integrating experimental structural and HTS data along with computational methods, this platform furnishes the identification of new scaffolds and binding modes often overlooked by traditional workflows. Such platform has potential for application to diverse targets and diseases contexts, while leveraging key Brazilian advantages: its rich biodiversity and CNPEM's capacity for generating large sets of experimental data.



CODETAC integrates high-throughput experimental data and computational modeling for drug discovery

Computational modelling applied to the discovery of new inhibitors of isocitrate dehydrogenase type 2 (IDH2).

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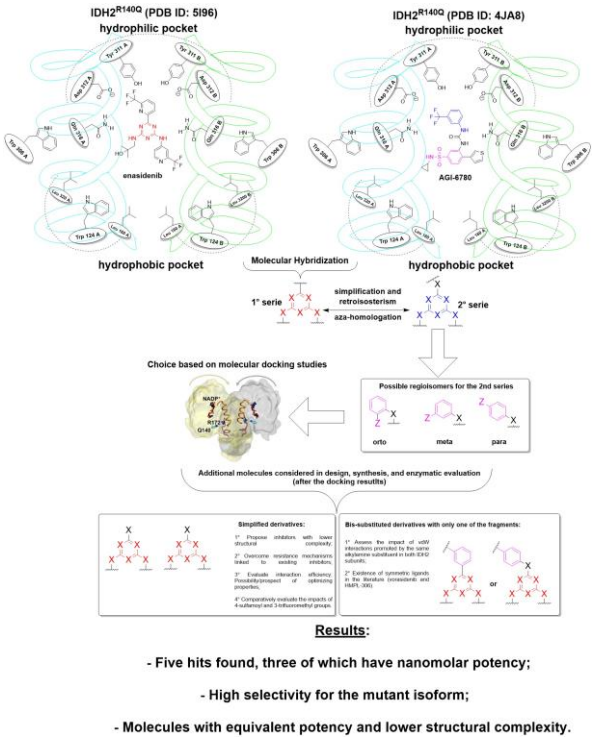
Palavras Chave:*MDGS,SBDD.,Isocitrate dehydrogenase,IDH2 inhibitors*

Highlights

Five compounds were identified as having a binding affinity for IDH2, three of which exhibited nanomolar potency. This result demonstrates the efficiency of MDGS and stimulates further studies.

Resumo/Abstract

Isocitrate dehydrogenase (IDH) has established itself as an emerging target in targeted therapies, mainly due to the approval of enasidenib in 2017 for the treatment of acute myeloid leukemia. However, this validation has not resulted in a growing number of discoveries, with only a few drugs approved since then and reports of loss of efficacy compared to current therapy. In this sense, the work carried out sought to contribute to the discovery of IDH2 inhibitors capable of overcoming these problems. To this end, two new series of molecules were designed, using selective inhibitors of mutant IDH2R^{140}Q (enasidenib and AGI-6780) as a structural framework, with the MDGS (Molecular Docking Guided Synthesis) approach — which is primarily based on data generated by molecular docking to guide the synthesis of new compounds — one of the methodological pillars of this research. Docking studies (performed using the Genetic Optimization for Ligand Docking (GOLD 2022.3) software) revealed molecules capable of interacting with key residues (**W164**,**I168**,**V164**,**V297**,**W306**,**V315**,**Y311, D312, Q316, I319, L320**) in the allosteric cavity of the IDH2R^{140}Q enzyme. Based on these results, molecules of lesser structural complexity (e.g., simplified derivatives) with equally relevant interaction profiles were also proposed. The molecules selected as potential candidates underwent preliminary evaluation of their pharmacodynamic (potency) and physicochemical (solubility and permeability) properties. In addition to proof of principle, the enzyme inhibition assays led to the discovery of five new selective hits for the IDH2R^{140}Q isoform, three of which had IC_{50} values in the nanomolar range (**44.15, 103.9 and 119 nM**), demonstrating the efficiency of MDGS in the search for new inhibitors. This discovery encourages the continuation of these studies, especially with a view to optimizing these derivatives (which are patentable) in order to broaden the therapeutic scope of AML.



Scheme summarizing the design, synthesis, and evaluation of new IDH2 inhibitors.

Agradecimentos/Acknowledgments

I would like to thank the funding agencies (CAPES, CNPq, FAPERJ), the analytical centers (LAMAR-IPPN and LBRMN-IQ), LASSBio, and UFRJ.

Conversion of α-lipoic acid into a dithiolated molecular platform for application as a multifunctional ligand.

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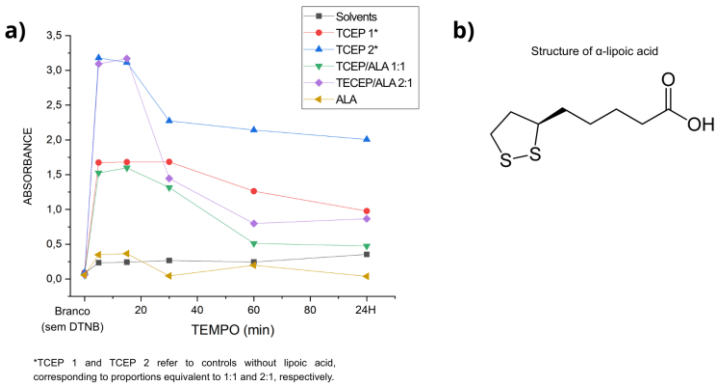
Palavras Chave:*α-lipoic acid, molecular platform, metallodrugs, multifunctional ligands.,α-lipoic acid, molecular platform, metallodrugs, multifunctional ligands.*

Highlights

The study evaluates the use of lipoic acid in coordination chemistry, highlighting its potential as a versatile molecular platform for the construction of multifunctional metal-based systems.

Resumo/Abstract

The modulation of the properties of metal complexes can be achieved through the use of multifunctional ligands capable of conjugating metal centers to bioactive units, enhancing stability, biodistribution, and biological activity[1]. α-Lipoic acid(ALA) is an endogenous compound found in living organisms[2] whose reduced form,dihydrolipoic acid (DHLA), contains free thiol groups that act as efficient metal coordination sites,making ALA a promising candidate for applications in coordination chemistry.Thus, ALA was investigated as a molecular platform for the development of gold(III)-containing complexes, evaluating its cytotoxicity and the reduction of intramolecular disulfides as a step toward generating dithiol species aimed at the formation of metal complexes. Cytotoxic effects were assessed in tumor (A549, B16F10) and normal (L929) cells.The results showed IC_{50} values higher than 100 µM, indicating the absence of cytotoxicity and supporting its application as a molecular platform. The reduction reaction of ALA was performed using tris(2-carboxyethyl)phosphine (TCEP) as the reducing agent and monitored by the 5,5′-dithiobis(2-nitrobenzoic acid) (DTNB) assay at 412nm(Figure 1).TCEP promoted DTNB reduction within approximately 10 min. In the presence of ALA, a progressive decrease in absorbance was observed, indicating consumption of the reducing agent and allowing the estimation that ALA reduction occurs within 60 min. The TCEP/ALA ratio influenced the reaction efficiency,with the 2:1 ratio being more efficient than 1:1. Control assays confirmed that oxidized ALA does not react with DTNB under the evaluated conditions, corroborating the role of TCEP and allowing estimation of the time required for generating free thiol groups suitable for coordination with gold(III). These results established conditions for in situ synthesis.As a perspective, this work aims to obtain gold(III) complexes with functionalized dihydrolipoic acid derivatives for pharmaceutical applications.



(a) ALA reduction by TCEP monitored by DTNB (412 nm) (b) Chemical structure of α-lipoic acid

Agradecimentos/Acknowledgments

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Democratizing Access to Bioactive Compound Data through a Curated USP Repository Integrated into the IRACEMA Project

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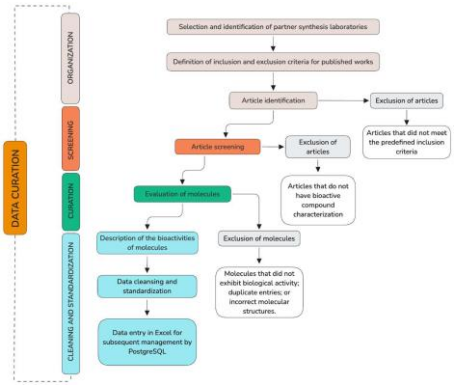
Palavras Chave:*Database,Bioactive Compounds,Data Curation,Drug Discovery,Chemoinformatics*

Highlights

Brazilian bioactive compounds database. Bioactive molecules from the University of São Paulo. Data integration and democratization of science

Resumo/Abstract

Bioactive compounds are chemical substances formed by two or more chemical elements that play essential roles in biological processes (NEWMAN, D. J.; CRAGG, G., 2020). According to an analysis report by Clarivate Analytics (2019), the University of São Paulo (USP) is the largest research center in Brazil, responsible for more than 20% to 30% of the national scientific production. However, this scientific production faces accessibility challenges for the general public. These challenges are related to the dispersion of scientific data, frequently presented in a heterogeneous, poorly standardized way and with restricted access (PILON et al., 2017). The construction of a library of bioactive compounds developed at the University of São Paulo aims to solve this problem, ensuring the democratization of scientific knowledge produced at the largest university in the country. For the curation of research data, sequential steps of organization, screening, curation, and standardization of data were established. The process begins with the selection and identification of partner synthesis laboratories, followed by the definition of inclusion and exclusion criteria applied to published works. From there, the identification and screening of articles takes place. The selected articles have their molecules validated, describing their bioactivity, followed by a data cleaning and standardization process, ensuring the consistency of the information. After this process, the data are entered and integrated into the IRACEMA project, a database management system for bioactive compounds isolated and characterized by Brazilian researchers. In this way, the library of bioactive compounds not only contributes to the democratization of access to scientific information, but also strengthens the IRACEMA project, expanding its database and promoting the integration of knowledge produced at USP and throughout Brazil.



Data Curation Process

Agradecimentos/Acknowledgments

We thank the Laboratory of Innovation in Therapeutics and Cheminformatics (LITEC) for its essential support, and all researchers and collaborators whose contributions to data collection and analysis were fundamental to this work.

Design and synthesis of 3H-imidazo[4,5-c]pyridine analogues against Leishmania infantum.

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Palavras Chave:*Bioactive compounds,Nitrogen heterocycles,Imidazopirydines*

Highlights

Novel benzimidazole and 3H-imidazo[4,5-*c*]pyridine analogues designed and synthesized as potential candidates against visceral leishmaniasis.

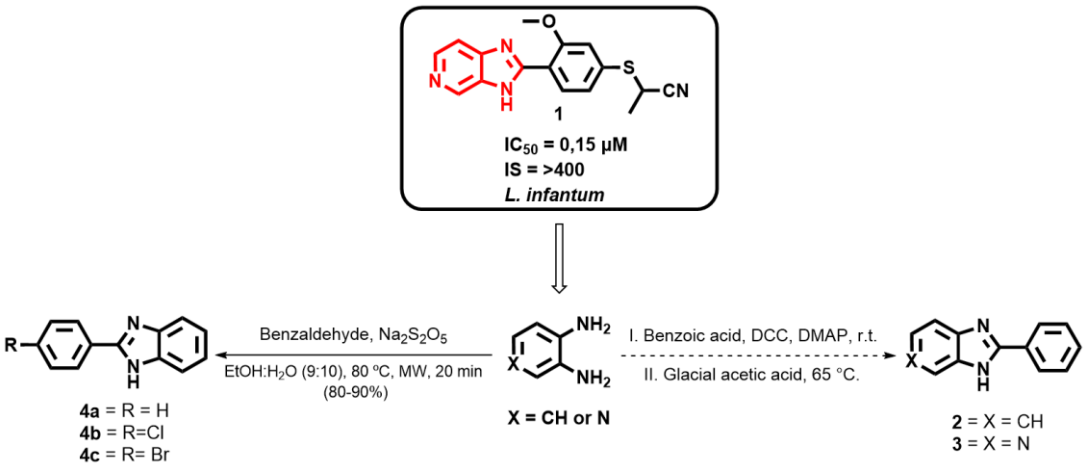
Resumo/Abstract

Neglected Tropical Diseases remain a global health challenge, particularly those caused by protozoa of the genus*Leishmania*. These infections are responsible for sever clinical manifestations, and still lack effective therapeutic options.[1] Visceral leishmaniasis, predominantly caused by*Leishmania infantum*in Brazil, is notable for the high toxicity, low efficacy and resistance of currently available treatments, highlighting the urgent need for novel chemical strategies in drug development.[2] The synthesis of a series of structural analogues, designed from a previously selected prototype (**1**) was proposed to be evaluated through structure-activity studies using rational medicinal chemistry strategies, such as molecular simplification. Synthetic routes has been proposed to aim compounds containing benzimidazole and 3*H*-imidazo[4,5-*c*]pyridine scaffolds. For benzimidazole analogues, a simple condensation of benzaldehydes and*o*-phenyldiamine under oxidative conditions under microwave heating was employed to afford the target compounds (**4a**–**4c**) within 20 min in high yields (80-90%), without the need for further purifications.[3] On the other hand, for 3*H*-imidazo[4,5-*c*]pyridine scaffold, milder conditions have been evaluated and are still under study, since the preliminary methodology employed did not afford satisfactory yields. These preliminary results showcase the feasibility of the methodology. Additionally, with one-step reaction affords the desired compound which enabling rapid expansion of the compound library.

[1] Berman,*Clinical Infectious Diseases*, 1997,**24**, 684–703.

[2] Guerin*et al*.,*The Lancet Infectious Diseases*, 2002,**2**, 494–501.

[3] Pham*et al*.,*RSC Adv*., 2022,**13**, 399–420.



Design and rapid synthesis of benzimidazole and imidazo[4,5-c]pyridine analogues

Agradecimentos/Acknowledgments

The authors gratefully acknowledge financial support from the São Paulo Research Foundation – FAPESP (2025/26719-9 and 2021/06661-5), and the Brazilian National Council for Scientific and Technological Development – CNPq (301771/2025-1).

Design, Synthesis, and Biological Evaluation of Cysteine Protease Inhibitors Targeting Cathepsin L and Cruzain

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Palavras Chave:*Cysteine proteases,Cruzain,Cathepsin L,Enzyme inhibition,Medicinal chemistry*

Highlights

- New inhibitors for cathepsin L and cruzain.
- Activity against targets linked to COVID-19 and Chagas disease.
- Improved binding through structural optimization.

Resumo/Abstract

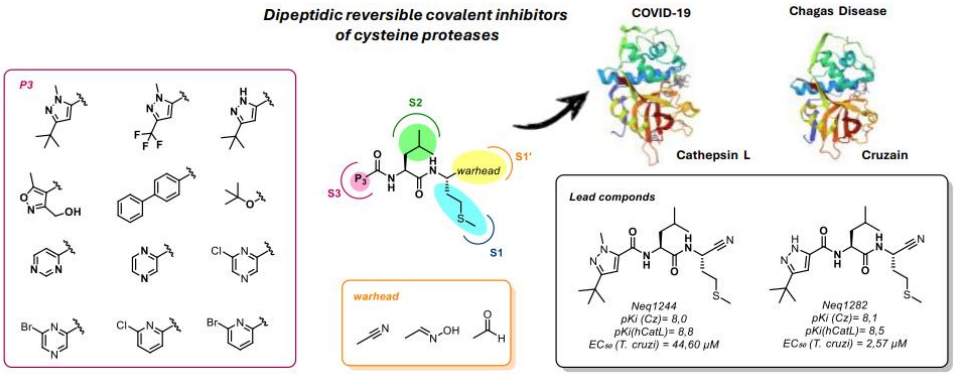
The therapeutic landscape for Chagas disease and COVID-19 remains limited by drug resistance and pharmacokinetic constraints of current treatments.[1],[2] Both diseases rely on homologous papain-like cysteine proteases, cruzain, essential for*Trypanosoma cruzi*survival, and human cathepsin L, involved in SARS-CoV-2 host cell entry.[3],[4] Exploiting this evolutionary conservation, we present an innovative, dual-application therapeutic strategy capable of inhibiting both enzymes. The core innovation of this study lies in the rational engineering of a novel series of fourteen dipeptidic reversible covalent inhibitors using a substrate-mimetic framework combining an electrophilic warhead with structural modulation at the S3 subsite. Biochemical evaluations revealed a remarkably flat structure-activity relationship (SAR) at the enzymatic level, with selected inhibitors achieving uniformly potent affinities (pKi > 8.0) against both cruzain and cathepsin L. This uniform biochemical affinity indicates that the reversible covalent interaction overwhelmingly drives initial active-site recognition. However, phenotypic assays showed variable antiparasitic activity against intracellular*T. cruzi*including EC_{50} from high to low-micromolar range, revealing that cellular potency is strongly influenced by modifications at the P3 position. The inhibitor Neq1282 is equipotent to benznidazole (EC_{50} = 3.98 µM) when used as a positive control. These findings demonstrate that while the electrophilic warhead secures dual-target enzymatic affinity, the optimization of the P3 architecture can be determinant for achieving robust intracellular exposure.

[1]**WHO.***Chagas disease.*2025.

[2]**WHO.***COVID-19 pandemic.*2025.

[3]**Duschak, V. G.; Couto, A. S.***Curr Med Chem.*2009.

[4]**Gomes et al**.*Front Cell Infect Microbiol.*2020.



Cysteine Protease Inhibitors for COVID-19 and Chagas Disease

Agradecimentos/Acknowledgments

The authors thank their research group colleagues for discussions and support. Financial support from CNPq, CAPES, and FAPESP is acknowledged. The Instituto de Química de São Carlos (IQSC–USP) is also thanked for infrastructure and facilities.

Design, Synthesis and Biological Evaluation of Hybrid JAK3/HDAC6 Inhibitors

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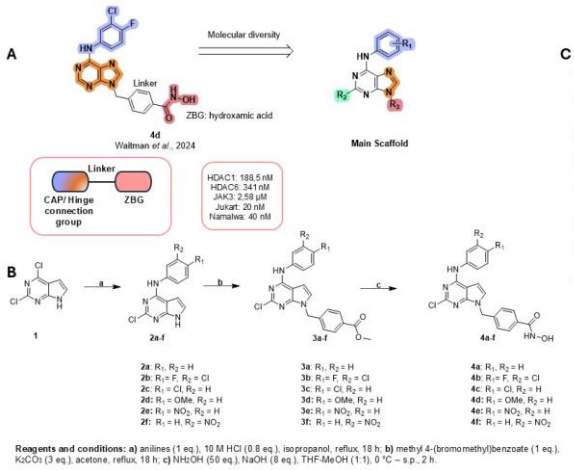
Palavras Chave:*Pharmaceutical Chemistry,Hematological cancer,Multi-target approach,Hybrid inhibitors,HDAC/kinase inhibitors*

Highlights

Deazapurine-based hybrids for dual HDAC6/JAK3 inhibition, using a hybrid scaffold strategy targeting epigenetic and kinase pathways in hematologic malignancies through rational bioisosteric design.

Resumo/Abstract

Polypharmacology has emerged as an effective strategy for the treatment of multifactorial diseases such as cancer. In this context, our laboratory (LAPESSB) previously developed hybrid HDAC and kinase inhibitors, which exhibited nanomolar potency against HDACs and micromolar activity against JAK3, showing antitumor activity at 40 nM in hematological tumor cell lines and a favorable pharmacokinetic profile. HDAC6 and JAK3 are enzymes associated with tumor proliferation and therapy resistance in hematological malignancies, including leukemias and lymphomas, which often show limited responses to conventional treatments. Based on the scaffold of coumpound**4d**(**Figure 1A**), this project aims to develop hybrid inhibitors capable of simultaneously modulating both enzymes. Using a bioisosteric approach, the purine core was replaced by a deazapurine nucleus to improve electronic and metabolic properties and enhance molecular interactions. According to the synthetic route presented (**Figure 1B**), the intermediate derivatives**2a–f**were successfully obtained through step (a), involving the reaction of the precursor with different anilines, resulting in the systematic introduction of the aromatic substituents R_1 and R_2. To date, these compounds have been obtained as shown in**figure 1C**, with isolated yields ranging from 47% to 75%. These derivatives constitute the structural basis for further molecular diversification and the development of hybrid inhibitors.



C

Compound	Yield (%)
2a: R_1, R_2 = H	51
2b: R_1= F, R_2 = Cl	71
2c: R_1 = Cl, R_2 = H	47
2d: R_1 = OMe, R_2 = H	63
2e: R_1 = NO_2, R_2 = H	53
2f: R_2 = H, R_2 = NO_2	75

*Yields obtained in triplicate

Design, synthesis, and yields of deazapurine-based hybrids targeting dual HDAC6/JAK3 inhibition.

Agradecimentos/Acknowledgments

The authors are grateful to Faculty of Pharmacy of University of São Paulo, which allowed the development of this work, CAPES, for financial support and grants #2024/22137-2 and #2024/07723-2 from FAPESP.

Development and application of a new flow-based method for screening acetylcholinesterase inhibitors

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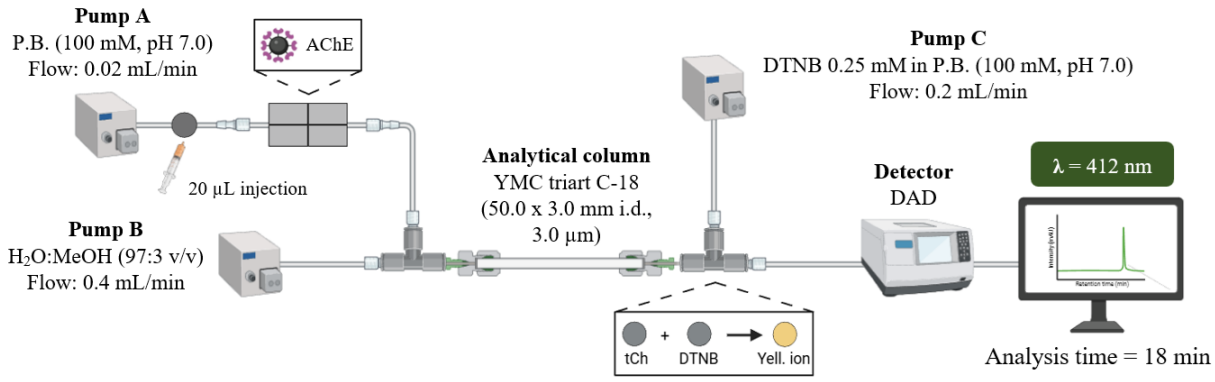
Palavras Chave:*Alzheimer's disease,Enzymes,High performance liquid chromatography,Inhibitory potential,Screening assays*

Highlights

AChE was immobilized onto magnetic particles, and its activity was monitored on-flow by HPLC-DAD. The developed activity assay was successfully applied to the screening of synthetic AChE inhibitors.

Resumo/Abstract

Alzheimer's disease (AD) is a highly prevalent, multifactorial neurodegenerative disorder for which currently available drugs present limited efficacy and significant adverse effects[1]. According to the cholinergic hypothesis, decreased acetylcholine levels resulting from the action of acetylcholinesterase (AChE) are directly associated with cognitive decline and disease progression[2]. In this context, this study describes the development, validation, and application of a new analytical method for screening AChE inhibitors. The enzyme was covalently immobilized onto iron oxide magnetic particles via glutaraldehyde crosslinking[3], enabling efficient reuse and improved analytical performance. Enzymatic activity was monitored by HPLC-DAD using an Ellman-based approach to quantify the yellow ion formed during acetylthiocholine hydrolysis. An on-flow chromatographic method was established using a C18 column with detection at 412 nm under optimized analytical conditions. Method validation followed ANVISA RDCs No. 166/2017 and No. 27/2012, demonstrating adequate linearity, selectivity, precision, accuracy, and reproducibility. Operational stability and reaction parameters confirmed the robustness of the immobilized enzymatic system. Kinetic analysis showed a*K*M constant of 1.02 ± 0.33 mM, consistent with immobilized enzyme systems. Screening of 16 coumarin-benzothiazole hybrids (with donepezil as control) identified two AChE inhibitors with IC_{50} values of 8.04 ± 1.71 and 9.00 ± 2.90 µM, and their inhibition mechanisms and*K*i constants were determined. Thus, this work presents a rapid, practical, robust, and reliable analytical platform for AChE inhibitor screening, contributing to the identification of potential drug candidates for AD treatment. References: [1] ZHENG, Q.; WANG, X.*Protein Cell*, v.16, n.2, p.83-120,**2025**; [2] GOULART, P. N. et al.*Rev. Virtual Quím*., v.13, n.1, p.90-126,**2021**; [3] XIMENES, I. A. T. et al.*J. Chromatogr. A*, v.1663, p.462740,**2022**.



HPLC-DAD on-flow conditions with in-flow thiocholine derivatization (P.B. = phosphate buffer).

Agradecimentos/Acknowledgments

FAPERJ, CAPES and CNPq

Development and biological evaluation of RD01-loaded nanostructured lipid carriers against Trypanosoma cruzi

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Palavras Chave:*nanostructured lipid carriers,triazole,Trypanosoma cruzi*

Highlights

Nanostructured lipid carriers loaded with RD01 showed high encapsulation efficiency, low cytotoxicity, and superior trypanocidal activity compared to the free compound against*Trypanosoma cruzi*.

Resumo/Abstract

Chagas disease, caused by the protozoan*Trypanosoma cruzi*, is a neglected tropical disease marked by decades of underinvestment in research and therapeutic innovation, resulting in limited and outdated treatment options associated with high toxicity. In this context, pharmaceutical nanotechnology emerges as a promising strategy to optimize the performance of trypanocidal compounds with biopharmaceutical limitations. A triazole compound, RD01, which is active against*T. cruzi*but exhibits low water solubility, compromising its efficiency in predominantly aqueous physiological environments, was previously developed. Thus, this study aimed to develop nanostructured lipid carriers (NLCs) containing RD01 and to comparatively evaluate their trypanocidal activity in relation to the non-encapsulated compound.

The formulation exhibited a mean particle size of 172.15 nm, determined by dynamic light scattering (DLS), with a polydispersity index of 30.12% and high encapsulation efficiency (95%). Cell viability and redox metabolism assays demonstrated that both blank nanoparticles and RD01-loaded nanoparticles did not interfere with mammalian cell viability, indicating adequate biocompatibility of the system. In antiparasitic assays, nanoformulated RD01 showed an EC_{50} of 28 µg/mL against the epimastigote form of the Y strain of*T. cruzi*, which was lower than that observed for the free compound (EC_{50} = 50 µg/mL). CC_{50} values were 297 µg/mL for the formulation and 280 µg/mL for free RD01, indicating low cytotoxic potential. Overall, the results demonstrate that RD01 nanoencapsulation preserves cellular safety and enhances trypanocidal activity, highlighting NLCs as a promising strategy for the treatment of Chagas disease.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPERJ

Discovery of dual-target ligands for cholinesterases from Moringa oleifera using affinity selection-mass spectrometry assay

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Palavras Chave:*Cholinesterase,AS-MS,affinity assay,natural products,dual-target*

Highlights

AS-MS enabled rapid dual-target cholinesterase ligand discovery. The approach accelerates natural product screening for Alzheimer's targets.*Moringa oleifera*is a source of dual cholinesterase ligands.

Resumo/Abstract

The development of new drugs is costly and challenging, especially for neurodegenerative disorders such as Alzheimer's disease (AD), which affects around 55 million people worldwide.[1] AD is characterized by cholinergic dysfunction and cognitive decline. Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) degrade acetylcholine and act as complementary therapeutic targets, with AChE predominant in early stages and BChE increasing as the disease progresses.[2] The limited efficacy of current inhibitors highlights the need for dual-target strategies. Natural products are promising sources of bioactive compounds, however, screening complex extracts is challenging. Affinity selection-mass spectrometry (AS-MS) enables rapid identification of target-binding ligands.[3] In this study, AS-MS was applied using AChE and BChE immobilized on magnetic particles to screen flower, stem, and leaf extracts of*Moringa oleifera*. Enzymes were incubated with extracts (2 mg/mL) for 30 minutes at room temperature. After magnetic separation, unbound compounds were removed, and high-affinity ligands were eluted with methanol (S3) and heated methanol at 70 ºC (S4). A control assay using inactivated enzymes evaluated non-specific binding. Ligands were analyzed by LC-HRMS, revealing selective dual-target compounds. Some were annotated using the GNPS platform (Table 1), while others are under identification using spectral databases and literature. The affinity ratio (AR) was calculated and only ligands with AR ≥ 1.20 were considered potential binders. Overall, AS-MS proved to be an efficient approach to accelerate the screening of ligands from*M. oleifera*against cholinesterases (ChE). After structural elucidation, the most promising compounds will be evaluated for inhibitory activity against ChE.

References

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RT (min)	*m/z*	AR (AChE)	AR (BChE)	Annotation	Extract
8.38	593.1515	1.79	1.27	nicotiflorine (ou kaempferol 3-*O*-rutinoside)	Leaf
8.76	609.1466	1.94	1.40	rutin	Flower

Table 1. LC-HRMS/MS analysis in negative mode and structure annotation for the identified ligands.

Agradecimentos/Acknowledgments

FAPERJ, CAPES, CNPq and PPGQ-UFF

Dithiocarbamate Derivatives Targeting Breast and Lung Cancer

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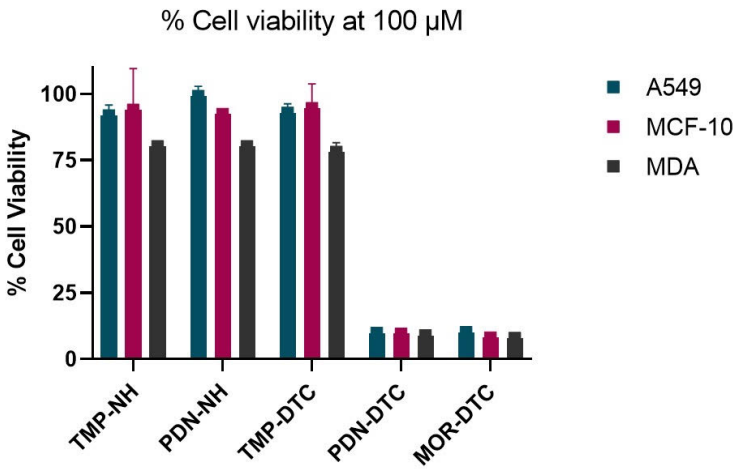
Palavras Chave:*cytotoxicityantitumoral,sulfur,cyclic,cytotoxicity,antitumoral*

Highlights

Three dithiocarbamate salts were synthesized and confirmed by NMR spectroscopy. Two salts showed cytotoxicity against breast and lung cancer cell lines.

Resumo/Abstract

According to the World Health Organization [1], cancer has affected over 19 million people in 2022, resulting in nearly 10 million deaths worldwide. The search for novel antitumoral agents seeks compounds that can be active and selective, so that treatment has minimal adverse effects. In this context, dithiocarbamates (DTCs) are a versatile class of sulfur-containing compounds (-NCS_2) that have been investigated as antiviral, antimicrobial and anticancer agents. Their biological activity is associated with enzyme inhibition, modulation of reactive oxygen species (ROS) production in cancer cells, and their ability to form complexes with transition metals such as platinum, palladium and gold [2]. Three DTC salts were synthesized, by reacting the corresponding amines with NaOH and excess CS2, the morpholine (MOR-DTC) and piperidone (PDN-DTC) DTCs formed precipitates and were washed with diethyl ether, whilst the tetramethylpiperidone DTC (TMP-DTC) was obtained by evaporation of the reaction solvent. They were characterized by ^{1}H and ^{13}C NMR spectroscopy. Changes in chemical shifts and the appearance of the CS2 signal confirmed the formation of the DTC salts. The cytotoxicity assay was conducted with the three DTC salts and the precursor amines, using three cell lines: MCF-10a (non-tumoral mammary), MDA-MB-231 (mammary adenocarcinoma) and A549 (lung adenocarcinoma). While the precursor amines showed no activity against cancer cells, their conversion into dithiocarbamate salts (MOR-DTC and PDN-DTC) resulted in cytotoxicity toward both cancerous cell lines, as can be seen in the figure.
In conclusion, the DTC salts were obtained and characterized accordingly, showing promising potential as an antitumor agent. Additionally, these DTCs are being investigated as ligands for metal complexes, aiming to further enhance their anticancer potential.
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Cytotoxicity assay results for DTC salts and some precursor amines.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG and UFMG

Docking into the LOK: A Computational Exploration of the Serine/Threonine Kinase 10 Back-Pocket with GW830263A Analogues

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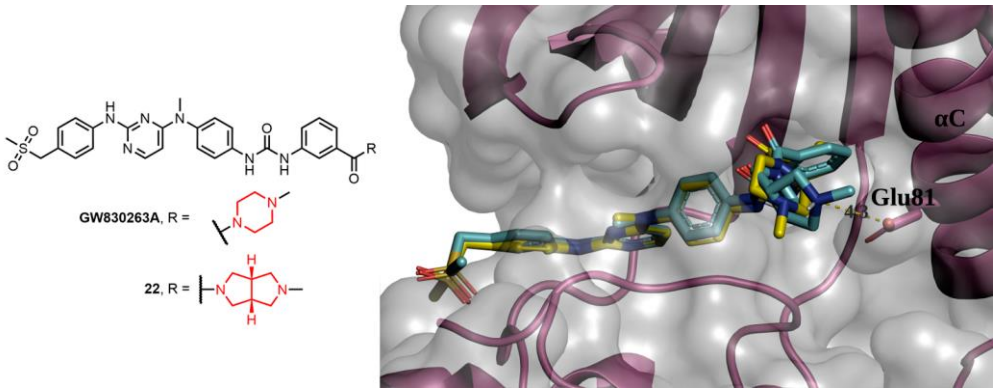
Palavras Chave:*serine/threonine kinase 10,kinase inhibitor design,molecular docking,bioisosterism,piperazine analogues*

Highlights

Novel LOK inhibitors designed through bioisosteric replacement of GW830263A piperazine moiety. Molecular docking identified fused analogue 22 with superior binding affinity.

Resumo/Abstract

Protein kinases (PKs) are regulatory enzymes governing most cellular processes through catalysis of reversible protein phosphorylation. PK dysfunction underlies cancer and other diseases, establishing these enzymes as critical therapeutic targets over the past two decades. However, nearly half of the human kinome remains chemically unexplored or underexplored, as evidenced by the scarcity of high-quality PK inhibitors. Serine/Threonine Kinase 10 (LOK, also known as STK10) represents an underexplored PK that activates ezrin/radixin/moesin proteins and regulates lymphocyte migration and cell cycle progression. Despite compound GW830263A binds LOK, as determined by X-ray crystallography, and has high affinity by DSF assays, no SAR exploration has been yet conducted. Therefore, leveraging the structural information on GW830263A binding mode, this work aims to design novel synthetically accessible hits by modifying the piperazine moiety with bioisosteric replacements. The crystallographic structure of LOK complexed with GW830263A was retrieved from the Protein Data Bank (PDB: 4AOT). Piperazine analogues from Enamine and Merck catalogs were employed for molecular modification. Ligand pKa values were calculated using MarvinSketch, and geometries were optimized in Avogadro with MMFF94s force field. Structures were prepared in AutoDockTools, and molecular docking was performed with AutoDock Vina following validation by redocking. Twenty-three analogues were evaluated, including spiro, bridged, and fused systems. Fused analogue 22 exhibited binding affinity (-12.9916 kcal mol^{-1}) slightly superior to the redocking control (-12.4386 kcal mol^{-1}). Visual inspection revealed that an electrostatic interaction between the protonated tertiary amine and glutamate (Glu81) of the αC-helix in LOK's back pocket may enhance ligand-receptor stabilization (Figure 1). This preliminary study selected analogue 22 for synthesis and subsequent biological validation of computational predictions.



1. GW830263A in yellow and 22 in cyan.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge financial support from the CAPES (GAS 88887.197241/2025-00), FAPESP (JCP 2021/06661-5), CNPq (JCP 301771/2025-1), Unicamp, URL and Department of Research and Universities of the Generalitat of Catalonia (RAMS).

Drug repurposing as a Multi-target approach in Alzheimer´s disease

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Palavras Chave:*Alzheimer's Disease, Drug Repurposing, Multi-target Drugs, Virtual Screening, Molecular Dockin,Alzheimer's Disease, Drug Repurposing, Multi-target Drugs, Virtual Screening, Molecular Docking*

Highlights

Multi-target strategy applied to Alzheimer's disease.

Drug repurposing using ligand- and structure-based virtual screening.

Identification of drugs with potential AChE, BuChE and GSK-3β inhibition.

Resumo/Abstract

Alzheimer's disease (AD) is a progressive neurodegenerative disorder and the leading cause of dementia worldwide, characterized by neuronal loss and cognitive decline. Its complex and multifactorial pathophysiology involves cholinergic dysfunction, β-amyloid accumulation, tau protein hyperphosphorylation, and neuroinflammation, which limits the effectiveness of therapeutic strategies based on single molecular targets.

Acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) play key roles in AD by regulating acetylcholine levels in the synaptic cleft. While AChE is predominantly expressed in the central nervous system and is directly associated with cognitive impairment, BuChE becomes increasingly relevant in advanced stages of the disease. In parallel, glycogen synthase kinase-3 beta (GSK-3β), a serine/threonine kinase, is strongly associated with AD progression due to its involvement in β-amyloid production, tau hyperphosphorylation, and neuroinflammatory processes. Considering the interplay among these targets, several multi-target compounds have been reported in the literature, including dual AChE/GSK-3β inhibitors, which have emerged as a promising therapeutic strategy for Alzheimer's disease.

In the present work, drug repurposing was performed using virtual screening campaigns combining ligand-based and structure-based methodologies. A curated drug database containing more than 8,000 compounds was compiled from different drug databases and repositories. The compounds were evaluated through molecular docking studies against AChE, BuChE, and GSK-3β in order to predict binding modes and interaction profiles. The virtual screening results allowed the identification of approved and investigational drugs with promising binding profiles toward more than one therapeutic target, highlighting their potential as multi-target candidates for Alzheimer's disease.

Agradecimentos/Acknowledgments

The author thanks**Prof. Dr. Carlos Henrique Tomich de Paula da Silva**for his guidance and the research group of the**Computational Laboratory of Pharmaceutical Chemistry**for their support in the development of this work.

Dual AChE/BACE1 Inhibition: Hybrid Structure- and Ligand-Based Screening of Dihydropyridines as Multitarget Alzheimer's Candidates

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Palavras Chave:*Alzheimer,dihydropyridines,acetylcholinesterase,Multitarget drug design,beta secretase 1*

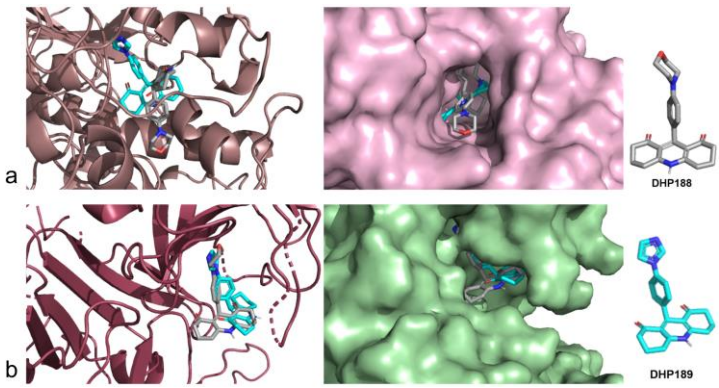
Highlights

An in silico hybrid strategy revealed dihydropyridine derivatives with multitarget potential against AChE and BACE1, key enzymes involved in Alzheimer's disease.

Resumo/Abstract

Alzheimer's disease is a progressive and multifactorial neurodegenerative pathology, motivating multitarget therapeutic strategies over the years, to modulate mechanisms involved in its progression[1]. In this context, dihydropyridines (DHPs) are promising scaffolds in Medicinal Chemistry due to their structural diversity and pharmacological relevance[2].
In this study, an in silico hybrid approach combining ligand- and structure-based strategies was employed to identify DHP derivatives with multitarget potential against acetylcholinesterase (AChE) and β-secretase 1 (BACE1) enzymes, related to the cholinergic and amyloid hypothesis[3]. Physicochemical properties of known ligands were evaluated using DataWarrior v06.05.02 to define acceptable ranges of molecular weight, cLogP, polar surface area, hydrogen bond donors/acceptors, and rotatable bonds, applied to a library of 756 compounds. Docking calculations were performed using AutoDock GPU on an NVIDIA GeForce RTX 4060 Ti (16 GB DDR6) against AChE (PDB ID:1CFJ) and BACE1 (PDB ID:6EQM) yielded average binding energies of −8.25 and −7.81 kcal/mol. Energy-based rankings identified the top 20 compounds per target; which 10 ligands appearing simultaneously were identified as potential multitarget.
Among these, compounds DHP_188 and DHP_189 showed relevant interactions with key amino acids of both enzymes (Discovery Studio Visualizer v24.1.0.23298), with average binding energies of −9.80 kcal/mol for AChE and −8.50 kcal/mol for BACE1. Molecular dynamics simulations using GROMACS will evaluate complex stability. The most promising compounds will be synthesized via Hantzsch multicomponent reaction[4] using corresponding aldehydes, dimedones, and ammonium for further characterization and biological evaluation.

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Docking overlap visualization of DHP_188 and DHP_189 in the enzymes a) AChE and b) BACE1.

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In silico identification of halogenated chalcones as potential Pseudomonas aeruginosa inhibitors

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Palavras Chave:*QSAR,Virtual Screening,Machine Learning,Genetic Algorithms,Antibacterials*

Highlights

Machine learning models, including SVM and MLP, demonstrate high predictive reliability. Virtual screening identifies halogenated scaffolds for experimental assays.

Resumo/Abstract

*Pseudomonas aeruginosa*is a multidrug-resistant pathogen requiring novel antibacterial agents. This study applies QSAR-based virtual screening to identify halogenated chalcones as potential*P. aeruginosa*inhibitors. Predictive models were developed using Support Vector Machine (SVM), Multilayer Perceptron (MLP), and linear regression algorithms, integrated with genetic algorithm-based descriptor selection. Models were validated through internal and external procedures, including Q^2, P^2, and Y-randomisation tests, to ensure predictive reliability. Performance variations across chemical subclasses highlighted specific structural patterns within halogenated scaffolds. A virtual screening workflow prioritised halogenated chalcones as promising hits. Distinct behaviour among halogen subclasses revealed structural differences influencing predicted activity profiles. The virtual screening workflow enabled the prioritisation of selected chalcone derivatives, which constitute promising candidates for subsequent experimental evaluation. These findings reinforce the applicability of QSAR-based strategies for guiding structure prioritisation in antibacterial research.

Agradecimentos/Acknowledgments

The authors thank the KNIME Team, FAPITEC/SE, CAPES, and CNPq for their essential support, provision of research grants, and the computational resources that enabled the development of this study.

In silico prospecting of Newbouldia laevis Seem. metabolites as NQO1 (4NWZ) modulators: identification of a bis-quinone scaffold

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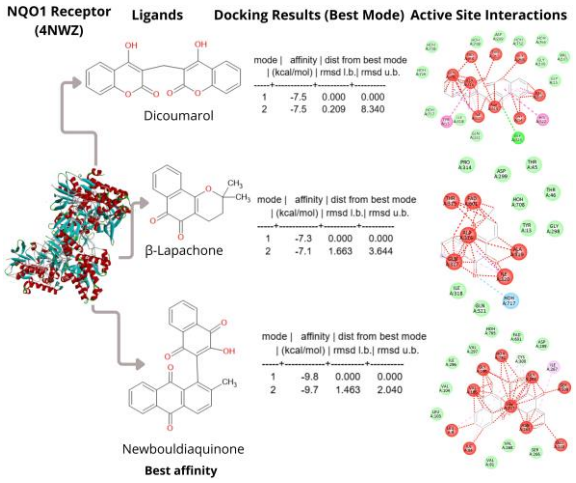
Palavras Chave:*Newbouldiaquinone,bis-quinone scaffold,computational medicinal chemistry,NAD(P)H:quinone oxidoreductase 1 (NQO1)*

Highlights

Novel bis-quinone scaffold; Newbouldiaquinone exhibits lower energy (-9.8 kcal/mol) than reference ligands and high affinity for NQO1; Demonstrates potential as an anticancer candidate

Resumo/Abstract

Newbouldia laevis Seem. is used in African ethnopharmacology, but is little explored internationally. This work presents an in silico study conducted in Brazil with metabolites of this species, aiming at the prospecting of modulators of NAD(P)H:quinone oxidoreductase 1 (NQO1), represented by the crystallographic structure 4NWZ, a flavoprotein present in progressive tumors. Overexpression of NQO1 is related to tumor cell survival and resistance to chemotherapeutic agents. Thirty secondary metabolites of N. laevis were selected from a systematic review using PRISMA 2020 methodology. The selected classes are naphthoquinones, terpenoids, and alkaloids. There is scientific evidence that some of these compounds exhibit antitumor activity, although action against NQO1 is not described, allowing for further studies. The software used were ChemSketch, Avogadro, PDB, ChemSpider, and SwissADME. Docking was performed in AutoDock Vina, AutoDockTools, and Discovery Studio. The active site was defined based on the FAD cofactor (FAD601) used as a structural reference and grid box (28 Å in x, y, and z). Dicumarol (energy of -7.5 kcal/mol) was adopted as the reference ligand because it is a competitive inhibitor, while β-lapachone (-7.3 kcal/mol) is the bioactive reference.
Six metabolites showed energies lower than the reference ligands; five were excluded for violating the Lipinski and Veber rules. Newbouldiaquinone stood out as the best ligand. It was the only molecule to meet the standards and present the lowest docking energy (-9.8 kcal/mol).
Dicumarol interacts through hydrogen and hydrophobic bonds, β-lapachone has hydrophobic interactions, and newbouldiaquinone has hydrogen bonds, π–π stacking, and hydrophobic bonds, combining moderate lipophilicity with polar interactions. The identified bis-quinone scaffold is not registered in public databases such as ChemSpider, reinforcing the innovative nature of the study.



Docking comparison of dicoumarol, β-lapachone and newbouldiaquinone at NQO1 active site binding

ESTUDO DE ESTABILIDADE E CARACTERIZAÇÃO FÍSICO-QUÍMICA DE NANOPARTÍCULAS pH DEPENDENTE CONTENDO TANINO CONDENSADO

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Palavras Chave:*nanoesfera,nanopartícula,caracterização,pH dependente,tanino*

Highlights

pH-dependent polymeric nanospheres encapsulating condensed tannins showed physicochemical stability over time, demonstrating potential for oral delivery.

Resumo/Abstract

Introdução: Taninos são polifenóis com alto potencial biotecnológico, podendo atuar na modulação da microbiota de animais, na inibição seletiva de patógenos e no controle parasitário. São frequentemente utilizados na suplementação animal. Entretanto, quando administrados pela via oral, complexam com as proteínas do trato gastrointestinal, influenciando negativamente na absorção de nutrientes. Com isso, busca-se o uso de nanocarreadores a fim de otimizar a administração de taninos. Nanoesferas poliméricas (NPs) são partículas maciças na escala nanométrica nas quais o fármaco se encontra na superfície da partícula ou disperso na matriz. De acordo com a escolha do polímero, as nanoesferas podem ser pH dependentes promovendo uma liberação controlada das moléculas associadas. Caracterizações físico-químicas subsequentes são relevantes para verificar a estabilidade da nanoformulação.**Objetivos:**Avaliar a estabilidade de tamanho, índice de polidispersão e concentração de partículas de NPs ao longo do tempo.**Método:**NPs preparadas com diferentes soluções-tampão e concentrações de tanino foram avaliadas em 1, 7, 14, 21 e 30 dias após o preparo. Observou-se visualmente a presença ou ausência de precipitados. As NPs foram caracterizadas em tamanho e índice de polidispersão (PDI) por espalhamento de luz dinâmico (DLS). A concentração de partículas foi medida por dispersão de luz dinâmica multiângulo (MADLS). O conjunto de dados obtidos foi tratado com o método estatístico ANOVA (análise de variância).**Resultados e conclusões:**Todas as NPs apresentaram tamanho na faixa nanométrica e PDI < 0,3, indicando homogeneidade dos sistemas. A concentração de partículas não apresentou tendência de oscilação entre os grupos. As NPs demonstraram tendência de diminuição de tamanho conforme aumento molaridade da solução-tampão neutra. Apenas as NPs com solução-tampão menos concentrada apresentaram alterações físico-químicas significativas indicativas de possível desestabilização do sistema.

Agradecimentos/Acknowledgments

Meus agradecimentos à agência de fomento FAPERGS, à Universidade de Ciências da Saúde de Porto Alegre e ao grupo de pesquisa TANANO.

ESTUDO IN SILICO DAS INTERAÇÕES PROTEÍNA-LIGANTE EM MAO-B POR ANÁLOGOS DA ISATINA PARA TRATAMENTO DE PARKINSON

Juliano Santos Reis (IC)*[1], Rosane Moura Aguiar (PQ)[1], Pedro Edson Moreira Correia (IC)[1], Isanna dos Santos Carvalho (IC)[1], Maria Paula Pereira Sousa (IC)[1], Martha Souza Vianna (IC)[1].

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Palavras Chave:*Monoamina oxidase B (MAO-B),isatina,docking molecular.*

Highlights

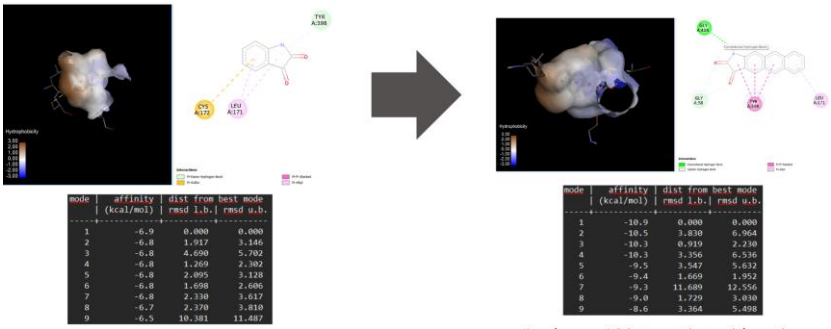
Molecular modeling of isatin. Eight of the twenty analogs are novel. Nineteen showed affinity greater than the ligand for the active site of MAO-B. The lowest energy found was -10.9 kcal/mol.

Resumo/Abstract

A Doença de Parkinson (DP) é um distúrbio neurológico associado a uma redução dos níveis de dopamina no corpo estriado. A monoamina oxidase B (MAO-B) é uma enzima mitocondrial que realiza o catabolismo da dopamina, sua inativação está associada ao potencial terapêutico na DP. Entre os inibidores de MAO-B, tem-se a isatina, uma molécula versátil, que se liga de forma reversível ao sítio ativo da enzima, resultando no aumento dos níveis de dopamina no cérebro. Portanto, o presente trabalho busca identificar derivados de isatina como novos potenciais inibidores da enzima MAO-B, aplicando ferramentas in sílico de docking molecular.

A estrutura cristalográfica da proteína (1OJA) foi obtida no site Protein Data Bank e a partir do estudo das interações (hidrofóbica, aromática e hidrofílica) da isatina com o receptor, vinte análogos foram desenhados a fim de aumentar sua afinidade. Alguns softwares foram utilizados, como o ChemSketch para desenhar os análogos e o Avogadro para otimização molecular. O Discovery Studio foi utilizado para analisar as interações ligante-proteína, enquanto o AutoDockTools serviu para preparar a enzima e os ligantes para o docking, que foi realizado com o AutoDockVina, com grid box de 20x20x20, para que os análogos se liguem na mesma região que a isatina.

De início, a isatina apresentou energia de ligação de -6,9 kcal/mol no sítio ativo. Dezenove análogos melhoraram a afinidade com a enzima, sendo o melhor (16) com energia de -10,9 kcal/mol. A principal alteração foi a adição de anéis aromáticos, que ajudou nas interações hidrofóbicas com o receptor. Também não houve violação das regras de Lipinski e Veber, critérios usados para prever a biodisponibilidade oral das moléculas, possuindo uma boa absorção gastrointestinal. 8 dos 20 análogos não apareceram na base de dados dos sites PubChem e ChemSpider, sendo moléculas inéditas. Em suma, os dados computacionais validam o potencial desses derivados de isatina como protótipos para o tratamento da DP.



mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-6.9	0.000	0.000
2	-6.8	1.917	3.146
3	-6.8	4.690	5.702
4	-6.8	1.269	2.302
5	-6.8	2.095	3.128
6	-6.8	1.698	2.606
7	-6.8	2.330	3.617
8	-6.7	2.370	3.810
9	-6.5	10.381	11.487

Isatin interaction with active site, binding energy and rmsd

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-10.9	0.000	0.000
2	-10.5	3.830	6.964
3	-10.3	0.919	2.230
4	-10.3	3.356	6.536
5	-9.5	3.547	5.632
6	-9.4	1.669	1.952
7	-9.3	11.689	12.556
8	-9.0	1.729	3.030
9	-8.6	3.364	5.498

Analogue 16 interaction with active site, binding energy and rmsd

Interações e energia de ligação da isatina e do seu análogo (16) com maior afinidade pelo receptor.

Agradecimentos/Acknowledgments

À UESB e à CNPq

Estudos Computacionais de bases de Schiff derivadas de ácidos m- e p-aminobenzóico e isatinas como potenciais fármacos contra Doença de Chagas

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Palavras Chave:*Bases de Schiff,Doença de Chagas,Triagem Virtual,Perfil ADMET,Docking Molecular*

Highlights

Chagas disease is one of the 20 neglected tropical diseases.
Treatment is restricted to two drugs with limited efficacy.
Schiff bases as new drugs for the treatment of Chagas disease.

Resumo/Abstract

A doença de Chagas (DC) é uma doença tropical negligenciada, devido ao baixo investimento em programas de desenvolvimento de novos fármacos, afetando cerca de 7 milhões de pessoas pelo mundo e seu tratamento é restrito a 2 medicamentos: o nifurtimox e o benzonidazol, introduzidos no mercado em 1967 e 1972, respectivamente. Contudo, ambos apresentam ineficácia em determinados estágios da doença, além de elevada toxicidade. Portanto, o desenvolvimento de novos fármacos que apresentem baixa toxicidade, boa eficácia e baixo custo são imprescindíveis, já que os investimentos para o desenvolvimento de fármacos para o tratamento da DC são limitados. Dado o exposto, uma metodologia promissora para o planejamento de fármacos é a triagem virtual, pois permite reduzir a quantidade de compostos a serem estudados, identificando os mais eficazes contra o alvo biológico. Assim, o objetivo deste trabalho foi realizar a triagem virtual de 12 compostos, por meio de docking molecular e análise do perfil ADMET, de Bases de Schiff (BS) derivadas de isatina e de ácidos meta- e para-aminobenzóicos, tendo em vista seu baixo custo e diversa atividade biológica, como potenciais fármacos para o tratamento da DC. Os resultados ADMET foram obtidos nos softwares SwissADME e Protox-III. Os resultados das BS estão dentro dos parâmetros estabelecidos por Lipinski. Além disso, elas apresentam probabilidade de atravessar a barreira gastrointestinal e estão nas classes 4 ou 5 de toxicidade, sendo aceitáveis para fármacos. O docking molecular foi realizado no software Gold, a enzima-alvo selecionada foi a cruzaína. A seleção dos melhores compostos foi feita com base nos scores da função de pontuação chemplp, juntamente com os melhores dados ADMET. As BS propostas apresentam perfil ADMET adequado, ademais, a atividade biológica foi averiguada de acordo com as interações com o sítio ativo. Sendo assim, as BS deste trabalho são promissoras como possíveis fármacos para o tratamento da DC.

Composto	Nome	N°. de violações (Lipinski)	Classe de Toxicidade	*Docking função ChemPLP*
	H-2	0	4	41,95
	H-3	0	4	43,38
	Me-2	0	4	41,59
	Me-3	0	4	42,25
	Cl-2	0	5	44,36
	Cl-3	0	5	43,52
	N-2	0	4	44,90
	N-3	0	4	44,07
	S-2	0	4	50,29
	S-3	0	4	52,89
	B-2	0	4	44,45
	B-3	0	4	49,61

Tabela das estruturas, siglas, dados ADMET e docking das bases de schiff

Agradecimentos/Acknowledgments

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Evaluation of acetylcholinesterase affinity toward donepezil and rivastigmine enantiomers in Alzheimer's disease treatment

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Palavras Chave:*Donepezil,Rivastigmine,Acetylcholinesterase,Molecular docking,Alzheimer's disease*

Highlights

Evaluation of acetylcholinesterase binding profiles of donepezil and rivastigmine enantiomers. Comparative docking analysis aiming at exploring stereoselectivity in acetylcholinesterase inhibition.

Resumo/Abstract

Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by cognitive decline and memory impairment, for which acetylcholinesterase (AChE) inhibitors remain among the most widely used therapeutic options. Donepezil and Rivastigmine are two clinically approved drugs that act by inhibiting AChE, thereby increasing acetylcholine levels in the synaptic cleft. Both compounds present chiral centers, and their enantiomers may exhibit distinct pharmacological profiles, including differences in binding affinity, selectivity, and therapeutic efficacy. Understanding the stereoselectivity of AChE inhibition is therefore crucial for optimizing drug design and improving treatment strategies in AD. It was performed a comparative analysis of the enantiomers of donepezil and rivastigmine through molecular docking simulations, with the objective to explore potential differences in binding modes, interaction energies, and stereoselective preferences of AChE toward each enantiomer. Although donepezil is marketed as a racemic mixture, the R-enantiomer shows a more favorable binding affinity profile toward AChE than the S-enantiomer. Docking analysis revealed interactions of the R-enantiomer with key residues within the AChE active site, including W72, W86, Y124, E202, S203, W286, Y337, F338, H447, and F295, with lower interaction energies and shorter binding distances, suggesting a more stable complex. With regard to rivastigmine, docking results showed that the S-enantiomer penetrates more deeply into the active site gorge, suggesting more favorable accommodation within the enzyme binding pocket. By employing molecular docking, this study offers insights into how chirality influences drug–target interactions, thereby providing a deeper understanding of the molecular basis of enantiomer-specific pharmacological effects.

Agradecimentos/Acknowledgments

The authors express their gratitude to the Military Institute of Engineering (IME) for providing the necessary infrastructure, and to CAPES, CNPq, and INCT-Defesa for their financial support.

Evaluation of Novel Ru(II)-p-Cymene Complexes their Anti-Proliferative Capabilities in Cancer Cell Lines and their Interactions with ct-DNA and BSA

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Palavras Chave:*Ruthenium,Anti-cancer,BSA,ct-DNA*

Highlights

Compound**IIIA**exhibits SI MRC-5/A2780 of over 25.

Both compounds exhibit electrostatic and hydrophobic interactions with ct-DNA and moderate interactions with BSA through a static quenching mechanism.

Resumo/Abstract

Cancer is defined as a large group of diseases which can originate in any organ or tissue of the body and is characterized by the uncontrollable proliferation of abnormal cells and are able to invade other organs and/or parts of the body. While several treatment options exist, one of the main options is chemotherapy. Patients all over the globe undergoing chemotherapy are often given cisplatin (derivatives), but these compounds fail in differentiating between cancerous and non-cancerous cells, they exhibit severe side effects and certain cancers evolved resistance to these compounds. Because of this, medicinal chemists are searching for new molecules to treat cancer. One of the classes of compounds being tested is the ruthenium (II) [Ru(II)] coordination compounds and have shown to be promising alternatives.

In this work, two novel Ru(II)-*p*-cymene compounds with the general formula [RuIICl(*p*-cymene)PR_3Pilo], with PR_3 being either PPh_3 (**IIA**) or tBuMePhos (**IIIA**) and Pilo being the pharmaceutical pilocarpine, their biological activity was evaluated. Their anti-cancer proliferation capabilities were evaluated*in vitro*among several cell lines, including A2780 using MRC-5 as the control. Selectivity indices greater than 25 were obtained for**IIIA**in the cell line A2780. Furthermore,**IIIA**its effects on cell morphology, cell colony formation and tumor size were evaluated*in vitro*using 2D and 3D cell assays. It was able to change the cells morphology from elongated to circular with increased cellular cohesion.**IIIA**was also able to inhibit colony formation as well as inhibit tumor growth.

Interactions of the compounds with calf thymus deoxyribonucleic acid (ct-DNA) and bovine serum albumin (BSA) were evaluated using fluorescence spectroscopy. Both compounds interact with ct-DNA through electrostatic and hydrophobic interactions. The compounds were able to interact with BSA with moderate association constants and fluorescence quenching through the static mechanism.

Agradecimentos/Acknowledgments

We would like to acknowledge CNPq, CAPES and FAPERGS (project 21/2551-0002119-5) for their financial contribution to this work.

Identification by Molecular Docking of a Novel Allosteric Subsite Useful for the Design of NMDA/GluN1–GluN2B Receptor Ligands

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Palavras Chave:*Molecular docking,Allosteric site,NMDAR/GluN1-GluN2B,Neurodegenerative disorders,Drug Design*

Highlights

Molecular docking study on NMDAR/GluN1-GluN2B allosteric site. Pharmacophoric descriptors provide evidence of novel subsite. Design of candidate drugs for the treatment of neurodegenerative disorders.

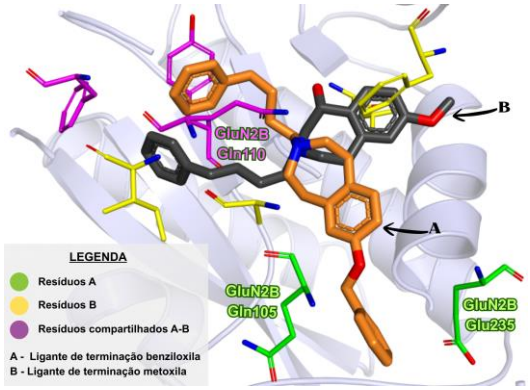
Resumo/Abstract

Glutamate receptors in the brain for which*N*-methyl-*D*-aspartate (NMDA) acts as a specific agonist are known as NMDA receptors (NMDARs). The development of NMDA receptor antagonists has been proposed for the discovery of drugs intended for the treatment of neurodegenerative diseases, such as Alzheimer's and Parkinson's diseases, as well as psychiatric disorders, including schizophrenia and bipolar disorder.

The NMDAR antagonists ifenprodil and EVT-101 interact at allosteric subsites well described in the literature. In this work, molecular docking of 239 NMDAR ligands, reported in the literature, was performed using the GOLD software (CCDC) at the allosteric modulation site of the GluN1–GluN2B NMDAR subtype. Molecular docking was performed within a 20 Å radius site around the Gln110B residue, at the center of the ifenprodil binding site. The analysis was based on pharmacophoric descriptors of the ligand–protein complexes and Pearson correlation, with data obtained from the Protein–Ligand Interaction Profiler (PLIP) tool.

This approach allowed the association of frequencies of interactions between ligands and binding-site residues. As a result, a previously unreported subsite within the allosteric site was identified, comprising residues Glu235B and Gln105B, which have not been described in the literature as part of the allosteric site. Benzazepine ligands were observed to interact differently with the allosteric site depending on their substituents; for instance, the benzyloxy group of a more potent ligand (Ki = 298 nM) interacted with these residues, whereas the interaction was absent in a less potent derivative bearing a methoxy group (Ki = 542 nM). These findings indicate that interactions at this new subsite enhance the binding to NMDAR.

Overall, this study reveals new interaction modes to be explored in SBDD models for the development of NMDAR ligand candidates, with potential applications in the treatment of neurodegenerative diseases and psychiatric disorders.



New pose (A) defining the proposed subsite, contrasting with the classic ifenprodil pose (B).

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Identification of Human Butyrylcholinesterase Ligands from Synthetic Natural Product Derivatives Using AS-MS.

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Palavras Chave:*AS-MS,butyrylcholinesterase,chromenes,curcuminoids,ligands*

Highlights

AS-MS as a powerful tool to accelerate the discovery of human BChE inhibitors; natural product–derived synthetic compounds.

Resumo/Abstract

Human butyrylcholinesterase (huBChE) is a key enzyme of the cholinergic system and presents increased activity in advanced stages of Alzheimer's disease, contributing to disease progression.[1] In this context, the identification of selective huBChE inhibitors presents significant therapeutic potential. In this work, an Affinity Selection Mass Spectrometry (AS-MS) strategy was applied to select ligands from complex mixtures and to investigate their inhibitory activity based on affinity ratio (AR) values. The AS-MS assay consists of immobilizing the target enzyme on a solid support, incubating it with the sample (S0), performing washing steps to remove non-specific ligands (S1–S3), desorbing high-affinity ligands (S4), and subsequently structural characterization[2]. HuBChE was immobilized on amino-functionalized magnetic nanoparticles via an amine–glutaraldehyde reaction, producing huBChE-MPs with immobilization efficiency and kinetic parameters consistent with literature data. The AS-MS platform was employed to screen two synthetic libraries: a mixture of ten 2-amino-4*H*-chromene derivatives (compounds J, MIX1) and ten monoketone curcuminoids (R1–R10, MIX2)[3]. Mass spectrometric analysis of the S4 fraction revealed the presence of four ligands from MIX1 and two ligands from MIX2. All selected compounds presented affinity ratio (AR) values greater than 1.0, indicating strong binding to huBChE. Enzymatic inhibition assays by using HuBuCh-IMERc- MS[4] demonstrated inhibitory activities ranging from approximately 46% (J1) to 68% (J11). The most active compounds will be further characterized through the determination of IC_{50} and kinetic (Ki) parameters.

Compounds	AR	Inhibitory activity (%)
J3	1.43 ± 0.26	59.01 ± 0.98
J5	2.75 ± 0.52	68.91 ± 2.59
J11	1.53 ± 0.17	46.92 ± 0.85
J15	1.46 ± 0.27	60.26 ± 0.09
R6	1.17 ± 0.01	65.19 ± 5.66
R9	2.05 ± 0.14	65.14 ± 2.01
Galantamine*	1.92 ± 0.87	83.29 ± 0.90

Table 1. Affinity ratios (AR) and inhibitory activities for ligands from synthetic natural products

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Identification of Prion Aggregation Modulators in Natural Products

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Palavras Chave:*Prion, Protein Aggregation, Affinity Selection-Mass Spectrometry, Ligands, Natural Products,Prion,Protein Aggregation,Affinity Selection-Mass Spectrometry,Ligands,Natural Products*

Highlights

Affinity Selection-Mass Spectrometry assay using PrP-coated magnetic particles applied to screen prion aggregation modulators.*Kielmeyera coriacea*leaf extract showed selective ligand retention.

Resumo/Abstract

Amyloidosis comprises a group of diseases characterized by protein aggregation into amyloid fibrils, which can accumulate in the brain and lead to neurodegeneration[1,2]. Prion diseases are rare, fatal disorders caused by the conversion of the cellular prion protein, PrPC, into its scrapie form, PrPSc, and exhibit a unique infectious mechanism, in which PrPSc can induce the misfolding of PrPC, resulting in accelerated progression and death[2]. Currently, there are no effective treatments for prion diseases, highlighting the need to identify molecules capable of modulating PrP aggregation. Herein, a real-time quaking-induced conversion assay was employed to screen the anti-aggregation activity of 11 natural product extracts. Afterwards, an HPLC-DAD method was developed to profile*Kielmeyera coriacea*leaf extract (KC-EEL). The method employed an INERTSUSTAIN C18 column (250 × 4.6 mm, 5 µm), with a mobile phase consisting of MeOH and 0.1% formic acid solution in gradient elution mode. Once the profile was established, an affinity selection-mass spectrometry (AS-MS) assay was conducted to identify ligands potentially associated with KC-EEL bioactivity. First, PrP was covalently immobilized onto magnetic particles (MP) functionalized with -NH_2 groups. Then, 500 µL of KC-EEL (3.0 mg/mL) was incubated with 2.5 mg of PrP-MP for 10 min. After magnetic extraction, the supernatant (S0) was removed, and the PrP-MP were washed twice, yielding S1 and S2. Ligand dissociation was performed by incubating the PrP-MP with MeOH for 3 min, generating S3. A control assay was conducted using Blank-MPs. Then, KC-EEL and supernatants from both assays were analyzed by UHPLC-HRMS using the developed method adapted for LC-MS. The AS-MS assay showed selective retention of 6 PrP ligands, with affinity ratios between 1.2 and 1.9. Currently, virtual libraries such as GNPS and Sirius are being used for structural annotation.[1]Amorim, M.*et al*. ACS Omega,**2025**; [2]Masone, A.*et al*. Neural Regen. Res.,**2024**

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Identifying candidate inhibitors of Trypanosoma cruzi proteasome from LASSBio chemical library by molecular docking and molecular dynamics

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Palavras Chave:*Molecular docking, Proteasome, Chagas disease, Molecular dynamics, Virtual screening*

Highlights

Molecular docking virtual screening with LASSBio chemical library and molecular dynamics analysis revealed candidate ligands of*T. cruzi*proteasome.

Resumo/Abstract

Chagas disease, caused by the protozoan*Trypanosoma cruzi,*affects approximately six to seven million people worldwide and leads to over 10,000 deaths annually[1]. Currently, benznidazole and nifurtimox are the only drugs approved for the treatment of Chagas disease.[1]The proteasome, a multi-subunit enzyme essential to the ubiquitin-proteasome system, represents a promising target for drug development. While some proteasome inhibitors are already approved for cancer treatment**,**others are being explored for neglected tropical diseases such as leishmaniasis, Chagas disease and sleeping sickness[2]. This study aimed to: I) Conduct a virtual screening of compounds from the LASSBio chemical library to identify potential new*T. cruzi*proteasome inhibitors.II) Perform molecular dynamics of proteasome complexes of selected compounds to evaluate their dynamic stability. The virtual screening was conducted with the subunit 20S of*T. cruzi*proteasome (PDB code 9F9T)using 1.931 compounds from the LASSBio chemical library. The protocols described in the FLARE program[3] were followed for molecular docking and molecular dynamics.The RMSD value found in a docking validation procedure was satisfactory(0.28 Å,below 2.0 Å, PDB code 6TCZ).In the virtual screening, compound LASSBio 458 achieved the best ΔG value, indicating a higher affinity for the target (-12.02kcal/mol), followed by LASSBio 340 (-11.69kcal/mol) and LASSBio 559 (-11.59kcal/mol)**.**In its best docking pose, LASSBio 458 formed hydrogen bonds with residues Tyr 223 and Gly239 from chain L and Tyr 25 from chain K. In addition, π-stacking interactions were observed with Phe24 e Tyr223. In molecular dynamics runsof the complexes,it could be observed adequate structural stability after 100 ns, with RMSD values between 2 and 4 Å,as exemplified in Figure 1 forthe best predicted ligand, LASSBio 458, and even for the tenth best one, LASSBio 558.

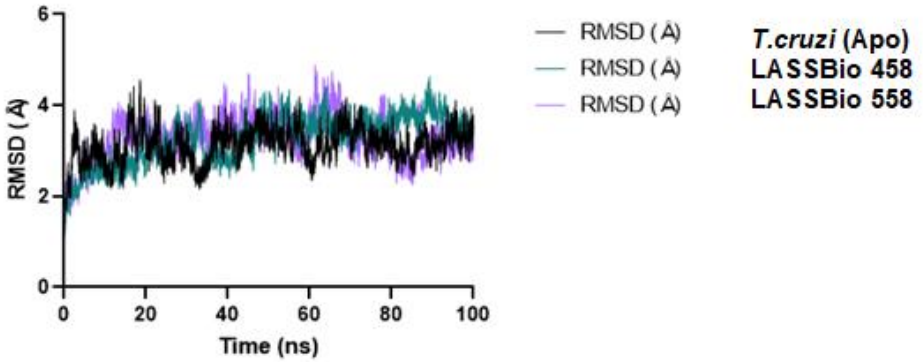


Figure 1: Comparison of the RMSD: T. cruzi proteasome, LASSBio 458, and LASSBio 558.

Agradecimentos/Acknowledgments

CAPES – CNPq – FAPERJ – INCT-INOFAR – LASSBio®

[1] WHO. Global Chagas Report**(2024)**; [2]EADSFORTH et al.,*J. Biol. Chem.*301, 108049(**2025**), [3]COUTSIAS et al., J. Comput.Chem.,25(15):1849,(**2019**).

In silico and in vitro evaluation of novel antiparasitic compounds targeting cruzain

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Palavras Chave:*Trypanosoma cruzi, Neglected tropical disease, Antiparasitic activity, Enzymatic Inhibition, TropMol*

Highlights

Investigation of the biological activity of compounds against the intracellular amastigote forms of T*rypanosoma cruzi*

Resumo/Abstract

Chagas disease is a neglected tropical disease that affects millions of people, primarily in developing countries, and is caused by the protozoan*Trypanosoma cruzi*(*T. cruzi*). It is estimated that the highest incidences are recorded in Latin America, where approximately 7 to 8 million people are infected, resulting in about 14,000 deaths per year. Despite being discovered over 100 years ago by the scientist Carlos Chagas, therapeutic options remain limited to only two drugs, which are associated with multiple adverse effects that frequently lead to treatment interruption[1]. One strategy to overcome these limitations is the development of targeted drugs that act on specific biochemical pathways, focusing on validated targets of*T. cruzi*. Among these targets, cruzain stands out, a crucial enzyme for the parasite's life cycle[2]. In this work, we searched for potential cruzain inhibitors by screening 10 compounds made available by the Medicines for Malaria Venture (MMV). These compounds were evaluated in silico using molecular docking to analyze enzyme-ligand interactions. Additionally, the TropMol-Caipora tool[3] was used to predict pIC_{50} values, enabling us to estimate enzymatic activity and identify promising candidates, with compounds 1 (pIC_{50} = 5.49) and 2 (pIC_{50} = 5.47) being highlighted. In the phenotypic screening of the intracellular amastigote form of the Tulahuen strain, we observed that compounds 1 and 2 exhibited moderate biological activity, with IC_{50} values of 16.9 ± 5.5 and 0.50 ± 0.11 μM, respectively. In the single-concentration enzyme inhibition assay, both showed inhibition greater than 50%. Therefore, these compounds can be subjected to structural modifications and further in vitro activity studies against cruzain.

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In Silico Pharmacokinetic Study and Structural Optimization of CauDHFR Inhibitors identified by Molecular Docking.

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Palavras Chave:*Antifungal,Hit Compounds,Drug Discovery,Virtual Screening,Pharmacokinetic Properties*

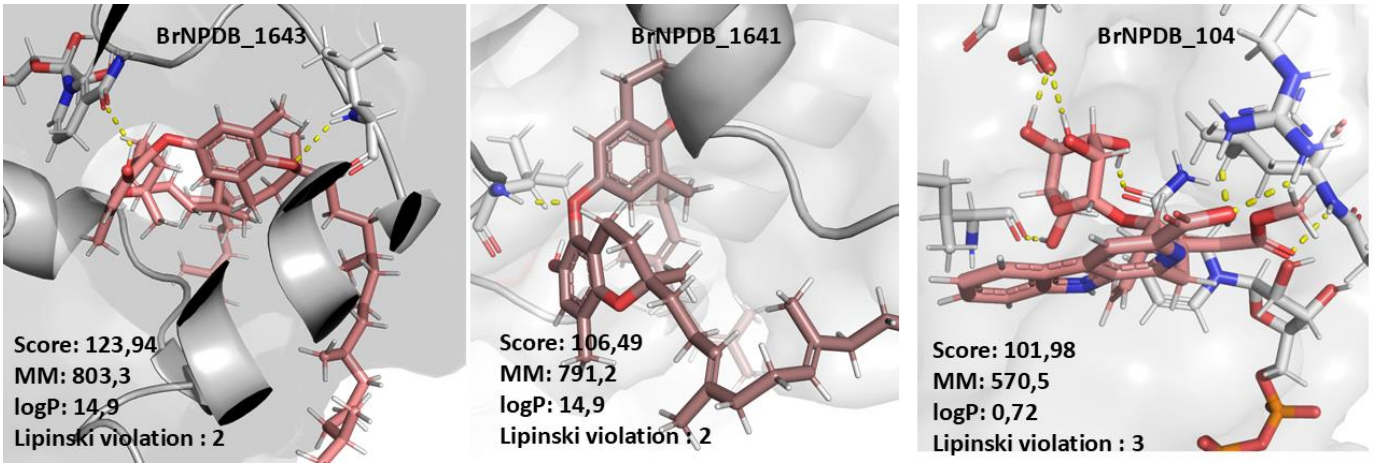
Highlights

Brazilian biodiversity provides natural products with antifungal potential against Candida auris, a drug-resistant pathogen. Targeting the DHFR enzyme in the folate pathway is a promising strategy.

Resumo/Abstract

Invasive Fungal Diseases (IFDs) are a category of infections caused by fungi that can affect internal organs and cause severe, often fatal, conditions. The rising incidence of these diseases is directly linked to the growing of increasingly resistant fungal strains. Using a Molecular Docking strategy for the analysis of the Brazilian Natural Product Database (BrNPDB), we selected 10 hit compounds with potential affinity for the active site of the enzyme dihydrofolate reductase from Candida auris (CauDHFR). This target is essential in the fungal folate pathway, making it a strategic choice against C. auris, a pathogen with high hospital incidence associated with severe systemic candidiasis. These infections contribute to a global scenario of approximately 1.5 million annual deaths caused by fungal infections. The integration of target-receptor interactions and pharmacological profiles, grounded in chemoinformatics tools, is a validated strategy for rational drug design. This approach enables more assertive screening, optimizing the drug discovery process by reducing costs and experimental time. In this study, in silico pharmacokinetic properties were determined using the SwissADME platform, evaluating parameters such as druglikeness, logP, molecular weight, polarity, insaturations (fraction Csp3), flexibility (nRotb), and solubility. Although the results indicate a limited pharmacokinetic profile, structural modifications were designed to optimize the biological performance of the molecules. These included molecular simplification and chain homology. Additionally, the effect of inserting polar groups are being studied to improve aqueous solubility and ensure that the selected molecules maintain adequate permeability across lipid membranes for future in vitro studies.

References: BAKCHI et al., 2022; BROWN et al., 2018; DENNING, 2024; KIM et al., 2024; SHOICHET et al., 2002; VALLI et al., 2013.



Molecular docking and pharmacokinetic profile of the hits.

Agradecimentos/Acknowledgments

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In silico prediction of protein allergenicity via Multilayer Perceptron networks and molecular descriptors based on amino acid sequences

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Palavras Chave:*Allergenicity,Machine Learning,Immunoinformatics,Chemoinformatics,Artificial Neural Networks*

Highlights

MLP model achieved 85.07% accuracy in external allergen validation. Low false-positive rate (9.65%) when screened against the human proteome. Sequence-based descriptors effectively classify allergens.

Resumo/Abstract

Protein-mediated hypersensitivity reactions represent a global epidemiological challenge, further exacerbated by the industrial requirement to introduce novel protein sources and the expansion of biopharmaceuticals and vaccines. Beyond food safety, identifying allergenic potential is vital for designing recombinant proteins, therapeutic antibodies, and vaccine antigens to prevent adverse immunological responses. Consequently, developing computational methods to predict immunogenic risk is crucial for public health. This study presents a predictive framework based on Multilayer Perceptron (MLP) neural networks for high-throughput identification of allergenic proteins. The positive dataset was consolidated from SDAP 2.0, COMPARE, AllergenOnline, WHO/IUIS, and Allergome. The negative control group was curated from UniProt using strict exclusion filters for allergenic and pathogenic properties. Numerical representation of primary sequences was achieved by calculating the mean value of each molecular descriptor ($D_{pr_{ot}}$) across constituent residues, normalised by the total sequence length (L). This was defined as the sum of the product of each standard amino acid frequency (f) and its corresponding descriptor value (d) divided by L. Descriptors were obtained via PaDEL-Descriptor. These features were subjected to a thorough selection pipeline involving low-variance filtering, collinearity analysis, and Logistic Regression. The MLP model demonstrated statistical robustness, yielding 85.07% Accuracy, 87.97% Sensitivity, and a 0.70 Kappa Coefficient in external validation. Furthermore, the model's discriminatory power was tested against the human proteome (n=15,539), exhibiting a low false-positive rate of 9.65%. Findings conclude that integrating molecular descriptors with MLP architectures provides a reliable, accurate screening tool for assessing biological safety across nutritional, pharmaceutical, and clinical sectors.

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In silico studies of isatin-derived Schiff bases as potential drugs against Chagas disease.

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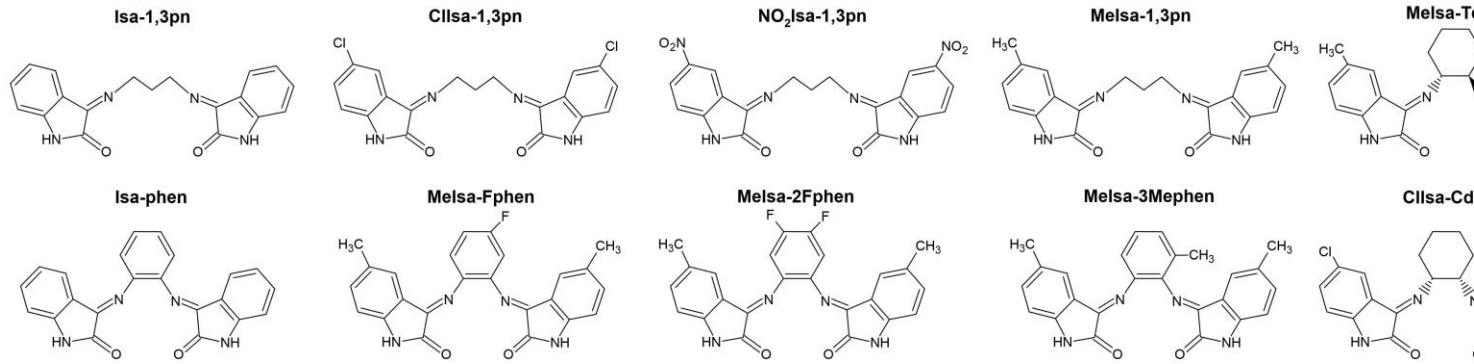
Palavras Chave:*Chagas Disease,Schiff Base,Isatin,molecular docking,ADMET studies*

Highlights

- Chagas Disease affects approximately 7 million people.
- Isatin-derived Schiff bases show potential as drugs against Chagas Disease.
- In silico analyses using ADMET studies and molecular docking.

Resumo/Abstract

Chagas disease is among the Neglected Tropical Diseases, mainly affecting poor populations in tropical and subtropical regions. Being a chronic, systemic, and parasitic infection caused by the protozoan*Trypanosoma cruzi*, it is estimated that approximately 7 million people are infected. Only two drugs are available for treatment: nifurtimox and benznidazole, both with adverse effects and effective only in the acute phase. Therefore, the need to develop new drugs is clear. In this context, CADD (Computer-Aided Drug Design) methodologies have been employed, which involves silico tests using computational tools. This reduces the time and cost of designing, selecting, and optimizing drug candidates. In this regard, Schiff bases have shown promising anti-Chagas activity due to their structural variability, which allows for the rational design of drugs with adjustable properties. Additionally, there is a growing interest in the development of new compounds from molecules with known biological activity, such as isatin. In this sense, this work describes a series of 56 Schiff bases derived from isatin, which were subjected to in silico analyses to evaluate their anti-Chagas potential. Molecular docking was used with the Gold 5.6 software, and ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity) studies were performed with the SwissADME and Protox-III software. The selection was based on the 10 compounds with the highest GoldScore values in the interaction with cruzain the molecular docking. Subsequently, in the ADMET studies, these were evaluated based on toxicity class between 4 and 5, non-violation of Lipinski's Rule, and suitability to bioavailability radars, which show promise for the development of new drugs against Chagas disease. Future studies will include in vitro evaluation of the selected compounds against cruzain.



Chemical structures of the 10 Schiff bases selected from in silico studies as potential anti-Chagas

Agradecimentos/Acknowledgments

Ao PPGNPMat-UFSC e à FAPESC pela bolsa concedida.

In silico study of tricyclic coumarins as prototypes for the treatment of Chagas disease

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Palavras Chave:*coumarins,flavonoids,drug,computational modeling*

Highlights

*In silico*evaluation identified tricyclic coumarins as potential virtual hits for Chagas disease

Molecular modeling against the*T. cruzi*Triosephosphate Isomerase enzyme showed favorable interaction

Resumo/Abstract

Introduction - Chagas disease (*Trypanosoma cruzi*) relies on treatments with severe adverse effects, requiring new alternatives. Tricyclic coumarins, based on natural anti-inflammatory scaffolds, represent versatile virtual structures for therapeutic applications. The parasite's Triosephosphate Isomerase enzyme is a strategic target for*in silico*evaluation. **Objective -** To evaluate 14 virtual structures modeled after synthetically viable tricyclic coumarins at the*T. cruzi*target enzyme's active site. **Methodology -** Virtual representations of the molecules (derived from the base scaffold shown in panel 1 of the Figure) were modeled in Spartan. Molecular docking was performed using Molegro Virtual Docker against the validated active site of the target enzyme structure (PDB: 4POC). **Results and Discussion -** Thirteen virtual structures exhibited lower predicted binding energies than the reference drug, benznidazole (-75.53 kJ/mol). Ten models shared predicted hydrogen bonds (blue dashed lines) with residues Arg100 and Gln147, similar to benznidazole (panel 2). Molecules 14 and 3 presented the lowest interaction energies (-125.01 and -111.63 kJ/mol, respectively). The superior stabilization of Mol 14 (panel 3) and Mol 3 (panel 4) is likely due to hyperconjugation effects, which enhance electron density distribution across the tricyclic system, allowing optimized anchoring. **Conclusion -** The evaluated virtual structures showed favorable theoretical interaction profiles. Given their synthetic viability, the most stable virtual hits (molecules 14 and 3) warrant future synthesis and*in vitro*validation to experimentally confirm these findings.

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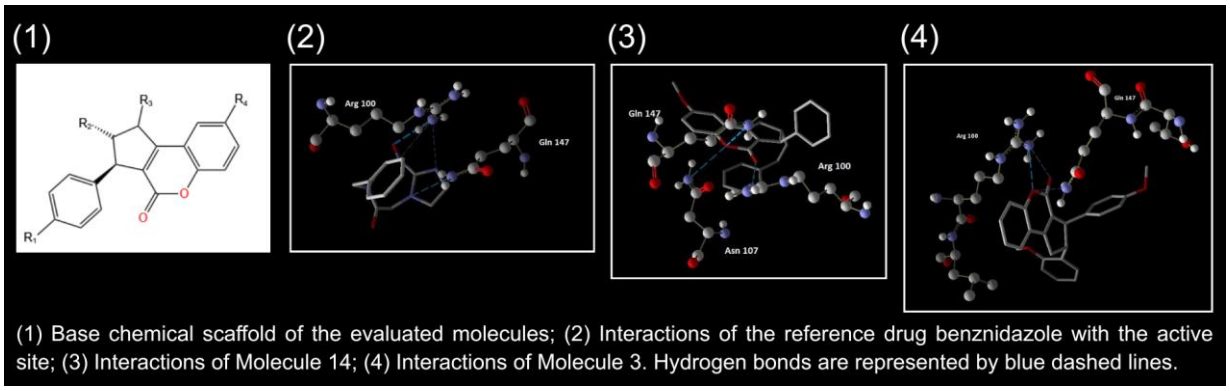


Fig 1: (1) Scaffold; Docking of (2) Benznidazole, (3) Mol 14, (4) Mol 3. Dashes: H-bonds.

Agradecimentos/Acknowledgments

We thank**Prof. Melissa Soares Caetano**for her guidance and**Prof. Jason Guy Taylor**for providing the compounds used in this research. We also acknowledge the support from the**Pró-Reitoria de Pesquisa, Pós-Graduação e Inovação (PROPPI/UFOP)**.

Integrated Molecular Modeling and Virtual Screening of Leishmania Sirtuin 2 Inhibitors

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Palavras Chave:*Comparative Modeling,Molecular Dynamics,Sirtuin 2-related protein 1,Molecular Docking,Pharmacophore Modeling*

Highlights

Sir2rp1 models from*Leishmania*were built by Comparative Modeling and refined by Molecular Dynamics. Pharmacophore Modeling and Molecular Docking were employed in a Virtual Screening of inhibitors.

Resumo/Abstract

Leishmaniasis are neglected diseases that affect more than 1.5 billion people around the world, mainly in developing countries, causing major socioeconomic impacts. The drugs available for the treatment of these diseases are ineffective and have several adverse effects. The process of researching new drugs involves the selection of biochemical targets essential for the survival of the causative agent. Sirtuin 2, an epigenetic enzyme essential for*Leishmaniaspp*parasites, is a validated target in the search for new drugs against them. Structure-Based Drug Design requires knowledge of the 3D structure of the target, thus structural elucidation and a detailed study of Sir2rp1 models from*Leishmania spp*is a valuable approach in the search for chemotherapeutic agents. This work applied Comparative Modeling using the Modeller software in the construction of Sir2rp1 models of the species*L. infantum*,*L. major*,*L. mexicana*,*L. amazonensis*and*L. braziliensis*. The constructed models were validated with basis on their stereochemical quality and folding. The enzymes' co-factor NAD^+ and the SirReal2 inhibitor were superimposed on the built models by structural alignment using the PyMol software and the validated complexes were subjected to Molecular Dynamics simulations using the GROMACS package. The refined complexes were then employed in the construction of Pharmacophore Models in the softwares MOE, LigandScout and Phase, and the consensus of the models was used to filter a curated small molecule database of approximately 9.3 million compounds. The selected 12 thousand compounds will be docked in the enzymatic models to select 100 to acquire and assay*in vitro*against the expressed enzymes. This work will pave the way for the development of safer and more effective leishmanicidal drugs.

GAO, Peng*et al.*Identification of Potent ADCK3 Inhibitors through Structure-Based Virtual Screening.**Journal of Chemical Information and Modeling**, v. 64, n. 15, p. 6072–6080, 12 ago. 2024.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPESP and FUSP

Investigação da redução de escala na produção de nanopartículas poliméricas pH-responsivas contendo SSIEFARL

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Palavras Chave:*Nanopartículas,Peptídeo,SSIEFARL,pH-sensível,Drug delivery*

Highlights

Otimização de nanoformulação com redução de volume final para aumentar concentração de SSIEFARL. Caracterização físico-química de formulação otimizada de nanoparticulas pH-responsivas.

Resumo/Abstract

A nanomedicina aplica a nanotecnologia à saúde por meio de materiais em escala nanométrica. As nanopartículas, devido à alta razão área/volume, interagem de forma mais eficiente com células, proteínas e fármacos. O grupo TANANO (UFCSPA) desenvolveu nanopartículas poliméricas (NPs) pH-sensíveis para administração do peptídeo SSIEFARL na mucosa genital feminina, visando tratamento imunoterápico contra HSV-2. As NPs foram preparadas por nanoprecipitação pH-dependente, método desenvolvido no grupo, utilizando polímero metacrilato (EUDRAGIT®), óleo de babaçu e tensoativos (Span® 80 e Tween® 80), e caracterizadas por DLS, MADLS e espalhamento eletroforético de luz (potencial zeta). Além disso, a formulação foi otimizada para obter-se maior concentração de SSIEFARL, reduzindo o volume final da formulação de 35 mL (F35) para 10 mL (F10), mantendo as proporções dos componentes, porém, observou-se alterações na caracterização da formulação otimizada. As análises foram realizadas em T0 e T30 (30 dias após a produção). O tamanho médio das NPs foi de 160 ± 4,7 nm em T0 e 171 ± 3,6 nm em T30 para F35, enquanto nas NPs da F10, há um aumento de tamanho já em T0 (172 ± 10,4 nm) e 189 ± 8,1 nm em T30. O potencial zeta diminuiu em módulo, de −11,9 ± 1,1 mV (F35, T30) para −8,37 ± 0,92 mV (F10, T30). Os valores de pH mantiveram-se semelhantes, em média de 1,2 ± 0,07, assim como os valores de PDI (F35: 0,18 ± 0,02 (T0) e 0,21 ± 0,02 (T30); F10: 0,163 ± 0,02 (T0) e 0,177 ± 0,03 (T30), porém, os gráficos de tamanho indicaram picos adicionais em F10, ausentes em F35, podendo significar formação de micelas de Tween® 80. Concluiu-se que a otimização foi bem-sucedida, sem evidências de instabilidade do sistema, entretanto, visando o futuro escalonamento da formulação, são necessários estudos adicionais e técnicas complementares de caracterização (DSC, FTIR, SAXS, entre outras) para elucidar a influência dos componentes e o impacto dessas alterações na estabilidade e responsividade das NPs.

Agradecimentos/Acknowledgments

.Agradeço imensamente à Universidade Federal de Ciências da Saúde de Porto Alegre, ao grupo TANANO e aos colegas do Laboratório de Farmacociências, à minha orientadora pelo apoio, ensinamentos e confiança, e ao CNPq e à CAPES.

Machine Learning Study of Negative Allosteric Modulators of the Metabotropic Glutamate Receptor 1 with Potential Applications in Alcohol Use Disorder

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Palavras Chave:*Ethanol,Machine Learning,Drug Discovery*

Highlights

Machine Learning study focused on negative allosteric modulators of mGluR1 for AUD. Curated ChEMBL dataset with decoys and clustering-based design. 1D/2D descriptors for robust predictive modeling.

Resumo/Abstract

Alcohol use disorder (AUD) is a major public health problem, with global per capita alcohol consumption of about 5.5 litres of pure ethanol in 2019 (World Health Organization, 2024), reinforcing the need for new treatments. Ethanol disrupts the balance between inhibitory GABA and excitatory glutamate signaling, causing acute depressant and rewarding effects, while chronic use induces neuroadaptations that contribute to tolerance, withdrawal, and compulsive use (Olsen; Liang, 2017).

The metabotropic glutamate receptor 1 (mGluR1) has emerged as a promising pharmacological target, where negative allosteric modulators (NAMs) of mGluR1 have been shown to reduce ethanol intake in rodent models (Lum et al., 2014). This study aims to identify and search for potential mGluR1 NAMs using machine learning methods. Potent mGluR1 inhibitors (IC50 ≤ 10 nM) were collected from ChEMBL, curated to remove redundancies, and used to calculate 1D/2D molecular descriptors with PaDel. Descriptors were filtered to exclude low variant, missing, and highly correlated variables.

To avoid biases in classification models, 20 decoys per active molecule were generated with DUDEZ and curated. Active molecules were clustered in KNIME using RDKit fingerprints and hierarchical and k-means methods, selecting the best clustering by silhouette coefficient. Based on these clusters, two datasets were assembled and split into training/test and external validation sets, with 4 decoys per active in each subset. 4 machine learning models were developed and validated to predict new mGluR1 NAMs with enrichment factors at 1% of 4.54 and ROC AUC higher then 0.98 for all models in both train/test and external datasets.

Agradecimentos/Acknowledgments

This work was carried out with support from CNPq (National Council for Scientific and Technological Development – Brazil), CAPES, and FAPESP.

Medicinal Chemistry of N-Benzyltryptamine Derivatives as Serotonin 5-HT2 Receptor Ligands

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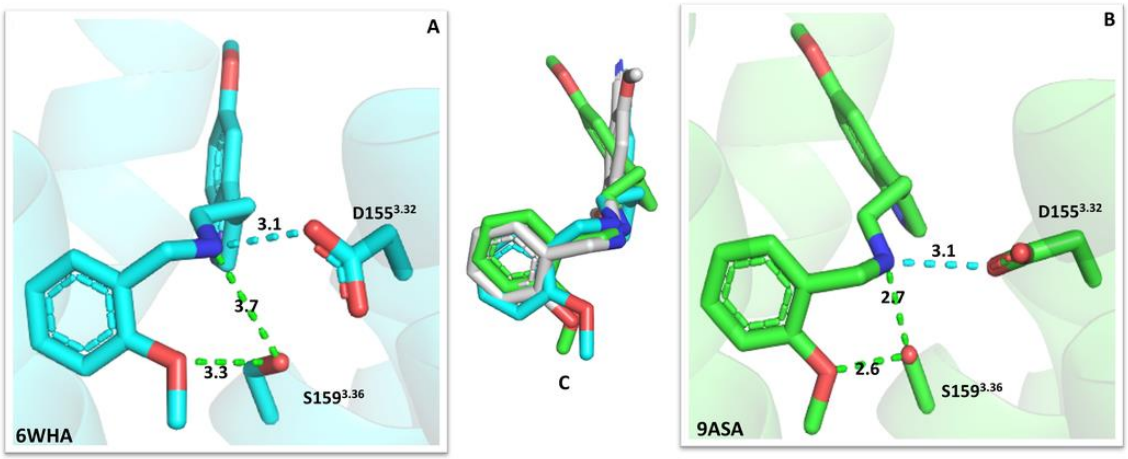
Palavras Chave:*N-benzyltryptamines, serotonin 5-HT2 receptors, radioligand displacement, QSAR, docking studies*

Highlights

N-benzyltryptamines evaluated as underexplored 5-HT_2 ligands. *Meta*substitution improves affinity, while*para*is detrimental. QSAR and docking explain SAR and highler activity of 5-methoxytryptamines.

Resumo/Abstract

Serotonin 5-HT_2 receptor ligands have attracted the attention of medicinal chemists for the last half-century, first as hallucinogens and later for their antipsychotic, appetite suppressant, antiaddictive and antidepressant potential. Unlike the very potent*N*-benzylphenethylamine derivatives that include the abundantly studied NBOMe drugs,*N*-benzyltryptamines have garnered little attention as potentially psychedelic serotonin 5-HT_2A receptor ligands, and none as possible leads for the development of novel agents for the treatment of cognitive disorders, substance abuse or depression. Here we have synthesized two parallel sets of 22 tryptamine and 22 5-methoxytryptamine derivatives bearing different unsubstituted and*ortho*-,*meta*- or*para*-substituted (OMe, Me, NO_2, F, Cl, Br, I)*N*-benzyl substituents and assayed them for their affinities and functional activities at the serotonin 5-HT_2A, 5-HT_2B, and 5-HT_2C receptors under identical conditions for each receptor subtype. In this way we have obtained highly comparable data allowing QSAR analysis to be performed which clearly showed the favorable effects of*meta*- and the unfavorable effects of*para*-substitution of the benzyl moiety. Considering the electronic and volumetric properties of the substituents, their effects could be attributed respectively to beneficial van der Waals forces in the*meta*position and steric clashes of para substituents. Docking simulations carried out on different ensembles of the active states of the 5-HT_2A receptor suggested possible explanations for the higher activities of the 5-methoxytryptamines, the preference for*meta*-substituted benzyl groups, and the relative inactivity of the*para*-substituted benzyl analogs.



Most potent compound 5MeOT-NB2MeO docked in two active-state ensembles of the 5-HT2A receptor.

Agradecimentos/Acknowledgments

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Microscale parallel synthesis and evaluation of pyrazolyl urea derivatives as potential antitrypanosomal agents

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Palavras Chave:*Microscale Parallel Synthesis, Antitrypanosomal, Neglected Tropical Diseases,Microscale Parallel Synthesis,Antitrypanosomal,Neglected Tropical Diseases*

Highlights

Microscale parallel synthesis and direct testing of crude reaction mixtures were applied to accelerate the hit-to-lead optimization of potential antitrypanosomal pyrazolyl urea derivatives.

Resumo/Abstract

Neglected Tropical Diseases (NTDs), particularly Chagas disease, Human African Trypanosomiasis, and Leishmaniasis, constitute a severe global health burden, affecting over one billion individuals worldwide. Currently available therapeutic options are limited by high toxicity, complex administration protocols, and the emergence of drug-resistant parasitic strains. This study addresses the the critical demand for novel chemotherapeutics by optimizing a pyrazolyl urea derivative that previously demonstrated moderate inhibitory activity against*Trypanosoma brucei rhodesiense*(IC_{50} = 8 µM) but suffered from poor aqueous solubility. To accelerate the discovery of potent analogues, a microscale parallel synthesis strategy was employed to explore the chemical space around the pyrazolyl urea scaffold. The urea derivatives were obtained through carbamoylation of the precursor 5-(pyridin-3-yl)-1*H*-pyrazol-3-amine followed by reaction of the intermediate with different amines. The latter stage was conducted at a micromolar scale in 96-well plates. The reactions yields and product purity were assessed by ^{1}H NMR and LC-MS. The crude mixtures of high yielding reactions (≥ 70 %) were submitted for phenotypic screening against*T. cruzi*,*T. brucei*, and*Leishmania spp.*, alongside cytotoxicity assays. The preparation of this focused library represents a strategic effort to streamline the transition from initial hits to optimized drug leads. Beyond identifying new compounds, this work demonstrates how a high-efficiency, small-scale production method can be applied for NTDs drug discovery. By combining chemical synthesis directly with biological testing, we bypass the slow and difficult purifying steps typically required, greatly speeding up our ability to test new ideas and understand how chemical changes affect drug potency.

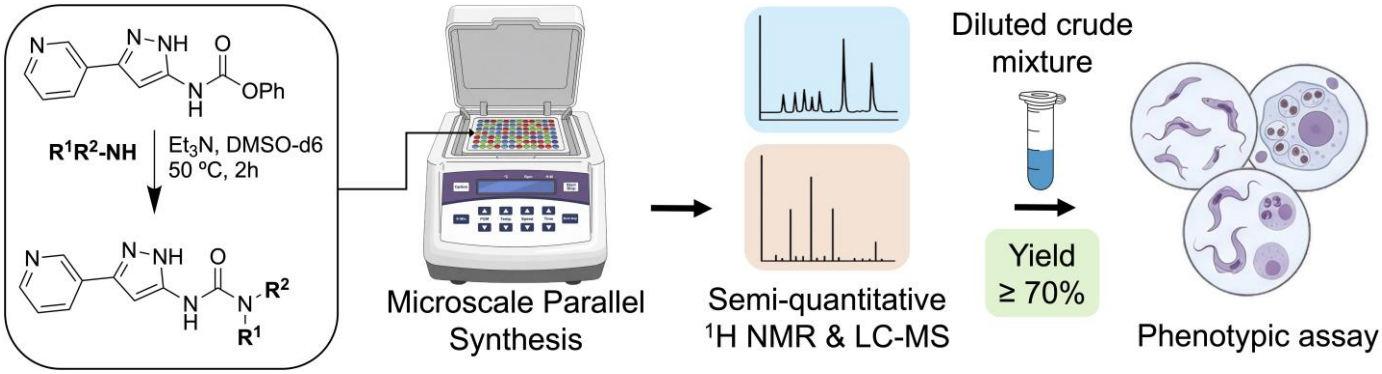


Figure 1. Workflow for microscale parallel synthesis and phenotypic screening of reaction mixtures.

Agradecimentos/Acknowledgments

We would like to thank the São Paulo State Research Foundation (FAPESP) for their financial support [process numbers: #2024/22131-4 (CVSC); #2024/08271-8 (DGS); #2023/11804-5 (DGS)].

Modificação estrutural de antifúngicos triazólicos: síntese de derivados do fluconazol e tebuconazol para estudo de mecanismo de resistência fúngica

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Palavras Chave:*Antifúngicos triazólicos,fluconazol,tebuconazol*

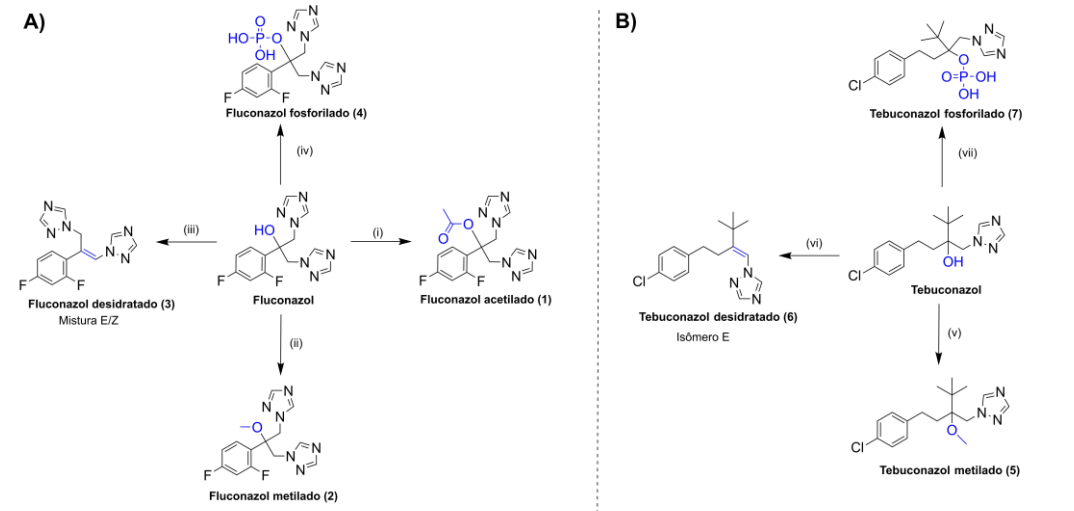
Highlights

Structural modification of azole antifungals via hydroxyl functionalization of fluconazole and tebuconazole. Evaluation of resistance fungal mechanism.

Resumo/Abstract

Os antifúngicos são essenciais no tratamento de infecções fúngicas em humanos, animais e plantas. Entretanto, o uso extensivo e contínuo desses compostos tem contribuído para a crescente resistência dos fungos, comprometendo a eficácia do tratamento e representando um desafio significativo para a clínica médica atual. Nesse contexto, compreender os mecanismos de defesa desses microrganismos que levam à resistência fúngica é fundamental para elucidar os processos envolvidos e desenvolver novos antifúngicos com maior eficácia. O objetivo desse trabalho foi a síntese de derivados dos antifúngicos fluconazol e tebuconazol, amplamente utilizados em medicina e agricultura, respectivamente. A obtenção desses derivados visou a avaliação de sua atividade antifúngica e à correlação entre modificações estruturais e potenciais mecanismos de resistência, contribuindo para a compreensão de como alterações químicas em antifúngicos podem impactar sua eficácia. As modificações realizadas envolveram a funcionalização da hidroxila terciária presente nos antifúngicos, por meio de reações de acetilação, metilação, desidratação e fosforilação, empregando metodologias clássicas. Na figura tem-se o esquema de síntese dos derivados, bem como os reagentes e condições. O derivado acetilado do fluconazol mostrou ser um importante composto envolvido no mecanismo de resistência fúngica de*Cryptococcus deuterogattii*e*C. neoformans*a este fármaco, sendo este o primeiro relato de inativação enzimática de fungicidas por fungos comprovado e descrito na literatura.1 Até o momento foram sintetizados quatro derivados do fluconazol (**1–4**) e três derivados do tebuconazol (**5–7**). A síntese dos derivados do fluconazol**2**e**3**, bem como dos derivados do tebuconazol**5**e**7**é inédita. Os compostos estão sendo avaliados quanto à sua atividade, visando a elucidação do papel de modificações estruturais na origem e no desenvolvimento da resistência fúngica.

1 Eufrasio et al.,*Drug Resist Updat*, 2026, 85, 101359.



Reagentes e condições:
A: i) Anidrido acético, NaH, DMF, 0 ºC → t.a., 48h, 80%; ii) MeI, NaH, THF, 0 ºC → 66 ºC, 5h, 91%; iii) 1- $SOCl_2$, $CHCl_3$, 70 ºC, atm. N_2, 2h, 2- Et_3N, CH_2Cl_2, 70 ºC, 20h, 76%; iv) $POCl_3$, Et_3N, DCM, t.a., atm. N_2, 48h, 91%.
B: v) MeI, NaH, DMF, 0 ºC → 70 ºC, 72h, 13%; vi) 1- $SOCl_2$, $CHCl_3$, 70 ºC, atm. N_2, 2h, 2- Et_3N, CH_2Cl_2, 70 ºC, 24h, 39%; vii) $POCl_3$, Et_3N, DCM, t.a., atm. N_2, 48h, 88%.

Esquema de síntese dos derivados do fluconazol (1-4) e tebuconazol (5-7).

Agradecimentos/Acknowledgments

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Multitarget Drug Repurposing Approach For Chagas Disease

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Palavras Chave:*Neglected Tropical Diseases,Chagas disease,Drug repurposing,Molecular Docking,Drug discovery*

Highlights

Multitarget molecular docking for the discovery of novel candidates for Chagas disease through a drug repurposing multitarget approach. Application of TropMol to predict cruzain inhibitors.

Resumo/Abstract

Chagas disease (CD) is a neglected tropical disease (NTD) caused by the protozoan*Trypanosoma cruzi*that affects more than 7 million people worldwide. Discovered in 1909 by Carlos Chagas, the disease still does not have safe and fully effective treatment options; benznidazole and nifurtimox both have severe drawbacks that often lead to treatment discontinuation (1). Therefore, there is an urgent need for novel and safer therapeutic alternatives. Drug repurposing is a strategy that can increase the success rate of drug development from approximately 1 in 10,000 to nearly 3 in 10, and has proven particularly effective for NTDs (2). Cruzain is a validated target for CD, as it plays an essential role in parasite survival (3). However, recent studies highlighted the difficulty of translating compounds active against cruzain into effective anti-chagasic agents (4). In this context, this work aimed to apply a multitarget drug repurposing approach. A library of 1,500 FDA-approved compounds was virtually screened against cruzain, trypanothione reductase, and dihydroorotate dehydrogenase. Docking was performed with GOLD using ChemPLP, the protocol was validated by redocking (RMSD < 2.0 Å) and ROC curve analysis (AUC > 0.80). Analysis of the top 10% ranked compounds for each target identified 61 compounds ranked across all three proteins (Figure 1). Using the TropMol-Caipora web tool to predict cruzain inhibitors (5), 48 of the 61 compounds were predicted to exhibit pIC_{50} > 5, representing a computational hit rate above 78% for cruzain. Future*in vitro*studies are necessary to confirm the biological activity of these compounds and validate the multitarget strategy for CD drug discovery.

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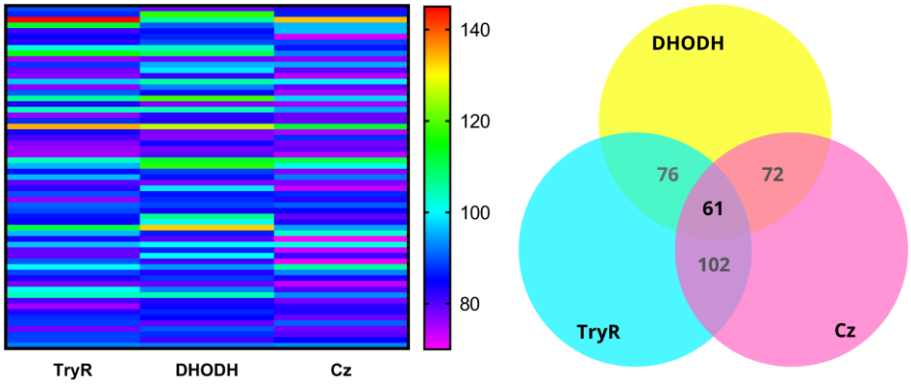


Figure 1 - Heatmap and Venn diagram of the results.

Agradecimentos/Acknowledgments

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New Cannabidiol-based Terpene N-Acyl-Aryl-Hydrazones with Potent Antinociceptive and Anti-Inflammatory Activity

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Palavras Chave:*Cannabidiol; CBD analogues; antinociceptive activity; anti-inflammatory activity; N-acyl-hydrazones.*

Highlights

Eight CBD-inspired terpene hydrazones were synthesized. PQM-242, PQM-243 and PQM-249 showed strong antinociceptive and anti-inflammatory effects. Lead compounds showed favorable ADME and no toxicity.

Resumo/Abstract

Inflammation is a protective mechanism of the organism in response to noxious stimuli, aiming to restore cellular homeostasis and tissue integrity. If the acute response fails, it may evolve into chronic inflammation, a key factor in the onset or progression of diseases such as cardiovascular disorders, rheumatoid arthritis, diabetes, cancer, COVID-19, and neurodegenerative diseases. The vanilloid receptor TRPV1 has emerged as a key player in pain modulation and a potential target for cannabidiol (CBD), a non-psychoactive phytocannabinoid that exhibits antioxidant, anti-inflammatory, antiepileptic, anxiolytic, and antidepressant effects. In this context, a novel series N-acyl-aryl terpene hydrazone derivatives was designed as simplified CBD-based analogues, leading to eight compounds (PQM-242 to PQM-249) synthed via a three-step route with global yields of 10–57%. All compounds were evaluated in vivo by the formalin and capsaicin-induced licking tests for antinociceptive and anti-inflammatory activity, aiming to confirm CBD-like effects and possible TRPV1 involvement. In the formalin test, PQM-242, PQM-243, PQM-244, PQM-248 and PQM-249 significantly reduced nociceptive behavior compared with control animals (63.7 ± 9.1 s neurogenic phase; 233 ± 30.2 s inflammatory phase). In the capsaicin model (56 ± 6.9 s in control), PQM-243 (10 µmol/kg) produced the strongest inhibition, surpassing capsazepine. As a result, PQM-242, PQM-243, PQM-244, PQM-248 and PQM-249 were identified as the best antinociceptive and anti-inflammatory candidates among the synthed series. The new CBD-based architecture reproduced the antinociceptive profile of CBD and showed adequate predicted ADME properties with no apparent toxicity, representing promising prototypes for the development of new analgesic and anti-inflammatory agents targeting TRPV1.
Referências:
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NMR-Based Development of a Fragment Library for Enzyme Ligand Identification

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Palavras Chave:*FBDD, Compound library, Knime Analytics NMR,FBDD,Compound Library,Knime Analytics,NMR*

Highlights

From chemical filtering to NMR validation: a custom-built fragment library for enzymatic ligand discovery.

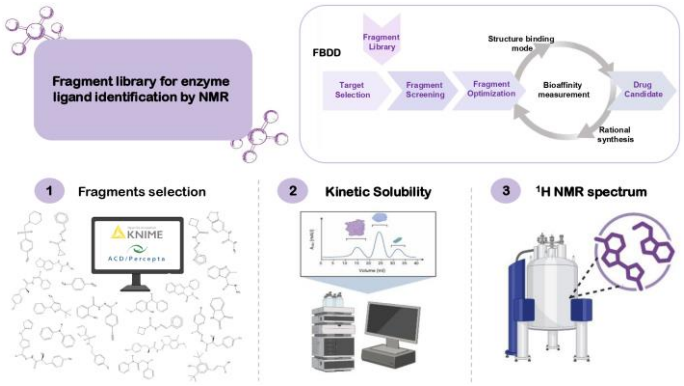
Resumo/Abstract

Fragment-Based Drug Design (FBDD) originated from the “SAR by NMR” method[1] and has been widely applied in the pharmaceutical industry, leading to the approval of drugs such as vemurafenib, sotorasib, and asciminib. This approach relies on low-molecular-weight fragments (< 300 Da) with low structural complexity and weak initial affinity for the biological target, which can be subsequently optimized. However, commercial fragment libraries are often associated with high costs and physicochemical limitations, such as low solubility and purity issues[2], particularly in academic research. In this context, the present work aimed to construct an in-house molecular fragment library for the identification of enzymatic ligands by nuclear magnetic resonance (NMR). The initial selection was carried out from the LASSBio compound collection, comprising 2,281 molecules, using KNIME Analytics software to apply the Rule of Three criteria, resulting in 64 fragments. These compounds were subsequently evaluated using Percepta (ACD/Labs) for lipophilicity (CLogP ≤ 3) and predicted solubility, leading to the selection of 31 fragments for experimental evaluation. The kinetic solubility of the fragments was assessed from DMSO stock solutions diluted in phosphate buffer, with assays performed in triplicate and incubation times of 4 and 24 hours. Samples were analyzed by high-performance liquid chromatography (HPLC) using a C18 column. Based on these results, a concentration of 100 µM was established as the standard condition for subsequent assays. Structural characterization and purity assessment were performed by ^{1}H NMR spectroscopy using Varian 400 and 500 MHz spectrometers. For the fragment LASSBio-1753, the spectra revealed the presence of two conformers in equilibrium, which was confirmed by variable-temperature NMR experiments. Additionally, spectra were acquired in phosphate buffer, allowing the evaluation of aggregation absence and the establishment of reference spectra for quality control.

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Workflow for fragment library design and experimental validation by NMR.

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OPTIMIZATION OF HYBRID HDAC6 AND JAK3 INHIBITORS BASED ON DEAZAPURINE-BENZO-HYDROXAMATES FOR THE TREATMENT OF HEMATOLOGIC MALIGNANCIES

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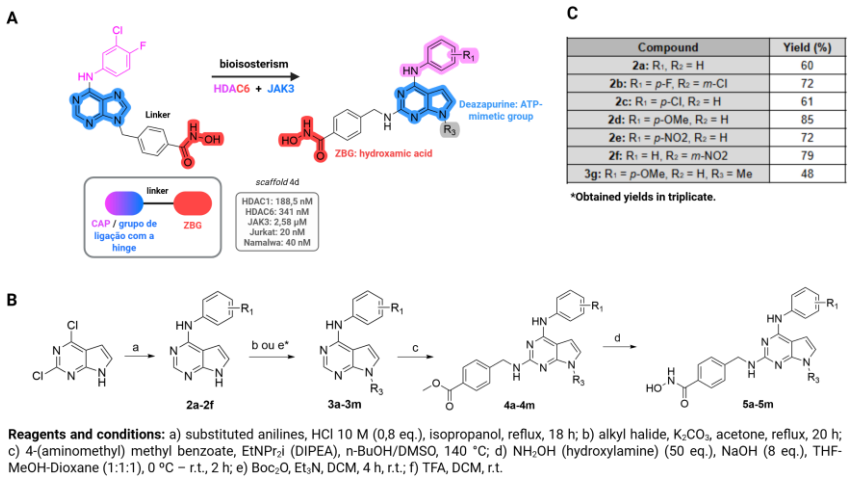
Palavras Chave:*Hybrid inhibitors, bioisosterism, HDAC6, JAK3, hematologic malignancies,bioisosterism, HDAC6, JAK3, hematologic malignancies,Hybrid inhibitors,bioisosterism,HDAC6,JAK3,hematologic malignancies*

Highlights

Deazapurine hybrids for dual**HDAC6/JAK3 inhibition**: rational**bioisosteric design**targeting epigenetic and kinase pathways. Single-scaffold strategy**selective against hematologic malignancies.**

Resumo/Abstract

HDAC6 and JAK3 are enzymes associated with tumor proliferation and therapy resistance in hematologic malignancies such as leukemias and lymphomas, which often show limited response to conventional treatments. Based on the scaffold of compound**4d**(**Figure 1A**), previously synthesized by the LAPESSB group, this project aims to develop hybrid inhibitors that simultaneously target both enzymes. Using the bioisosteric approach, the purine core was replaced by a deazapurine nucleus to improve electronic and metabolic properties and enhance molecular interactions. Structural modifications like variation in linker-ZBG position were designed to increase selectivity and efficacy. The synthetic route involves five steps (**Figure 1B**), and to date, compounds**2a–2f**(**Figure 1C**) have been obtained with overall yields of 31–85%, while compound**3g**was obtained in 48% yield.



Reagents and conditions: a) substituted anilines, HCl 10 M (0,8 eq.), isopropanol, reflux, 18 h; b) alkyl halide, K_2CO_3, acetone, reflux, 20 h; c) 4-(aminomethyl) methyl benzoate, $EtNPr_2i$ (DIPEA), n-BuOH/DMSO, 140 °C; d) NH_2OH (hydroxylamine) (50 eq.), NaOH (8 eq.), THF-MeOH-Dioxane (1:1:1), 0 °C – r.t., 2 h; e) Boc_2O, Et_3N, DCM, 4 h, r.t.; f) TFA, DCM, r.t.

Figure 1: A) Optimization of compounds; B) Synthetic route of compounds obtained; C) Purity and yiel

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Otimização da razão de soluções tampão na produção de nanopartículas poliméricas pH-dependentes

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Palavras Chave:*Nanopartículas,Nanomedicina,pH-responsivo,Química medicinal,Drug delivery*

Highlights

Otimização e caracterização de nanopartículas de Eudragit® FS 30D por ajuste da razão ácido–base, viabilizando a redução progressiva da molaridade final sem perda de estabilidade.

Resumo/Abstract

A nanomedicina permite desenvolver medicamentos e direcioná-los para regiões específicas do organismo por meio de formulações nanotecnológicas. O grupo de pesquisa TANANO (UFCSPA) desenvolveu partículas poliméricas (NPs) por uma metodologia de nanoprecipitação pH dependente, sem o uso de solventes orgânicos agressivos. Conforme o polímero empregado, as NPs adquirem caráter pH responsivo, permitindo o direcionamento da liberação da molécula associada. Neste projeto, investigou-se um novo polímero na preparação de NPs para encapsulamento de peptídeos. Buscou-se otimizar e caracterizar as NPs à base do polímero Eudragit® FS 30D, com ênfase na redução da molaridade final das NPs por meio da otimização da razão do meio tamponante ácido-base, visando evitar agregação, liberação inadequada e efeitos de*salting-out*. As NPs foram sintetizadas por nanoprecipitação pH dependente, contendo óleo de babaçu, polímero Eudragit® FS 30D, Span® 80, etanol, Tween® 80 e soluções tampão. As NPs foram caracterizadas quanto ao diâmetro, índice de polidispersão (PDI), potencial zeta, pH final da suspensão e ensaios de titulação avaliando a responsividade das NPs ao pH do meio. Verificou-se a viabilidade da produção de NPs com o novo polímero pela metodologia proposta.Essas apresentaram diâmetro médio de 180 nm ± 52; pH final médio de 0,7 ± 0,0; PDI médio 0,3 ± 0,0; potencial zeta médio -4,2 mV ± 1,3; aspecto homogêneo; o ensaio de titulação demonstrou a desestruturação das NPs em pH superior a 7. A molaridade final da dispersão foi 2,25 M. Com o novo polímero, diferentes formulações foram desenvolvidas por meio da redução da razão entre os tampões ácido e básico, visando diminuir a molaridade final das NPs. O tampão básico foi mantido constante, enquanto o tampão ácido foi reduzido para proporções 16, 8 e 5 vezes superior à do tampão básico, permitindo a redução da molaridade final sem perda da estabilidade das partículas, evidenciando o potencial da metodologia para reduções adicionais.

Agradecimentos/Acknowledgments

Os autores agradecem à UFCSPA pela infraestrutura disponibilizada e aos órgãos de fomento pelo apoio financeiro para a execução desta pesquisa.

Área:
MED

OTIMIZAÇÃO DE NANOPARTÍCULAS POLIMÉRICAS INOVADORAS PARA O CARREAMENTO E LIBERAÇÃO DE DICLOFENACO SÓDICO

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Palavras Chave:*Nanopartículas poliméricas,Diclofenaco sódico,Sistema de liberação,pH-responsivo*

Highlights

•Hydrophilic diclofenac sodium was encapsulated in pH-sensitive polymeric nanoparticles with optimized babassu oil core.

•Controlled release reached 76% in 24 h under physiological conditions.

Resumo/Abstract

As nanopartículas (NPs) são sistemas de drug delivery com diâmetro inferior a 1 µm, amplamente utilizados para otimizar a administração de fármacos. Entretanto, devido aos componentes comumente empregados em sua composição, esses sistemas apresentam maior afinidade por moléculas lipofílicas, o que limita a incorporação de compostos hidrofílicos. Diferentes métodos de preparação, como a nanoprecipitação, são empregados na produção de NPs. Foi desenvolvida pelo grupo uma formulação de NPs utilizando um polímero pH-responsivo e sem o uso de solventes orgânicos agressivos, possibilitando a incorporação de moléculas hidrofílicas. As nanopartículas foram otimizadas quanto ao aumento mássico do núcleo. Posteriormente, diclofenaco sódico foi incorporado na concentração de 0,5 mg/mL, o que não era possível na formulação original, e o sistema foi avaliado quanto ao perfil de liberação do fármaco sob condições semelhantes às fisiológicas. As NPs foram desenvolvidas pelo método de nanoprecipitação pH-dependente, utilizando óleo de babaçu, Span® 80, etanol, polímero metacrilato, Tween® 80 e soluções tampão. As nanopartículas foram caracterizadas quanto ao diâmetro, índice de polidispersão (PDI) e potencial zeta. Foram submetidas a estudos de liberação em pH 6,8, respeitando as características do polímero utilizado. Os ensaios foram realizados em triplicata, com coletas em 20, 30 e 45 minutos, 1, 2, 4, 6, 8 e 24 horas. As amostras foram analisadas por Cromatografia Líquida de Alta Eficiência, utilizando método previamente desenvolvido e validado. As NPs otimizadas, com aumento mássico de 0,011% de óleo de babaçu no núcleo em relação à formulação inicial, apresentaram diâmetro médio de 143 ± 2 nm, PDI de 0,23 ± 0,00 e potencial zeta de −3,2 ± 0,2 mV, resultando em partículas homogêneas, baixa polidispersão e estabilidade visual. O perfil de liberação foi contínuo e gradual, com liberação máxima de 76% em 24 horas, indicando resultados satisfatórios para o sistema proposto.

Physicochemical Characterization of a Nanoformulation and Its Incorporation into a Hydrogel for Vaginal Mucosal Delivery

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Palavras Chave:*nanomedicine;,hydrogel,chitosan*

Highlights

Optimization of a pH-dependent formulation for the biological pH of the female genital mucosa. Innovative production of a hydrogel containing 1% phosphoric acid and chitosan.

Resumo/Abstract

Nanoformulations exhibit adaptable physicochemical properties and potential as drug delivery systems for sensitive molecules. In this study, a hydrogel containing polymeric nanoparticles (NPs) was developed intended for vaginal mucosal delivery of a peptide. The NPs were prepared using the pH-dependent polymer EUDRAGIT® L30 D55 pursuing the intracellular delivery of the molecule. The pH of nanoformulations were adjusted with KOH (1 M) to the range 3.0–4.0 and characterized over 30 days in terms of size, polydispersity index (PDI), zeta potential, and pH. Titration assays were performed to evaluate the behavior of the pH-dependent polymer. Preliminary tests were also conducted using 5–6% chitosan combined with 2% acetic acid, 1% phosphoric acid, or solubilized directly in the nanoformulation to produce hydrogels. The size, PDI, zeta potential and pH of the nanoparticles after one day of preparation were 154 ± 2.7 nm, 0.28 ± 0.05, −13.3 ± 2.4 mV and 1.13 ± 0.06. The adjustment of the pH values to 3.0, 3.5 and 4.0 did not promote changes in NP over 30 days (T30) maintaining consistency among formulations. A reduction in PDI was observed at T30, indicating particle uniformity. The titration assay between pH 2 and 8, confirmed the responsiveness of the pH-dependent system. Near the deprotonation limit (pH ≈ 5.5) structural disruption of the particles was observed. The hydrogels were visually analysed and the pH were between 3-4. The hydrogel developed with 1 % phosphoric acid seems more suitable than the hydrogel containing acetic acid for vaginal application, since it was odorless and showed good visual solubilization of chitosan and nanoparticles incorporation. Further studies are being conducted to evaluate its rheological behavior, and more tests are needed to ensure the cytotoxicity and biocompatibility of the nanosystem.

Agradecimentos/Acknowledgments

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Piceatanol inhibits amyloid fibril formation during human hemoglobin glycation induced by fructose

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Palavras Chave:*Glycation,Amyloid fibrils,Piceatanol*

Highlights

Piceatanol reduced glycation-induced amyloid fibril formation in human hemoglobin systems with fructose, confirmed by ThT fluorescence, confocal microscopy, and DLS.

Resumo/Abstract

Glycation is a non-enzymatic reaction that occurs in biological systems and food matrices, involving reducing sugars, and nucleophilic groups of biomolecules[1]. The accumulation of advanced glycation end products (AGEs) has been associated with several pathological conditions, including neurodegenerative diseases such as Alzheimer's and Parkinson's[2]. Hyperglycemia promotes structural alterations in proteins, favoring misfolding and the formation of amyloid fibrils enriched in β-sheet structures[3]. In this context, this in vitro study aimed to evaluate the progression and inhibition of amyloid fibril formation during the glycation of lyophilized human hemoglobin using fructose (Fru) as glycating agents, and piceatanol (PIC; 10–300 µM) as an inhibitor. The experiments were conducted over a period of five weeks, and amyloid fibril formation was monitored by thioflavin T (ThT) fluorescence. Confocal fluorescence microscopy and dynamic light scattering (DLS) were employed to corroborate the fluorescence results and to analyze aggregate morphology and size distribution. The results demonstrated that PIC effectively inhibited amyloid fibril formation in a concentration-dependent manner. At 300 µM, PIC reduced fibril formation by approximately 52% in the Fru system. Confocal microscopy images confirmed a marked reduction in fibrillar structures using ThT probe, while DLS analysis indicated decreased particle size and aggregation. These findings indicate that piceatanol exhibits significant anti-amyloidogenic activity by modulating protein aggregation during glycation, highlighting its potential as a bioactive compound to mitigate glycation-induced protein misfolding and related disorders.

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PQM-250: a Pentamidine-based 1,2,3-Triazole-Hydrazone Analogue with Antileishmanial Activity against Leishmania (L.) amazonensis

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Palavras Chave:*Leishmania amazonensis, 1,2,3-triazole-hydrazones, Pentamidine, Antileishmanial*

Highlights

PQM-250 is a pentamidine-derived triazole-hydrazone analogue with potent antileishmanial activity. The compound exhibits low cytotoxicity and a favorable selectivity index (SI = 19.78).

Resumo/Abstract

Leishmaniasis remains a major public health concern in tropical and subtropical regions, where current therapies are limited by toxicity, variable efficacy, and parasite resistance. Pentamidine is known for its leishmanicidal activity; however, its clinical use is restricted by severe adverse effects, making it an important scaffold for molecular modification strategies aimed at developing safer and more selective analogues. In this context, a series of novel pentamidine analogue containing a 1,2,3-triazole–hydrazone core was evaluated, and PQM-250 was identified as the most promising compound. The new structural architecture was rationally designed through a structural modification approach based on the insertion of a 1,2,3-triazole subunit intended to modulate the biological and toxicological profile of the parent drug. PQM-250 demonstrated leishmanicidal activity against intracellular amastigote forms of*Leishmania (L.) amazonensis*(EC_{50} = 13.04 µM), whereas pentamidine showed an EC_{50} of 3.11 µM. Although less potent, PQM-250 exhibited low cytotoxicity in murine macrophages and a favorable selectivity index (SI= 19.78), indicating an improved balance between efficacy and safety and suggesting that the structural modifications contributed to a better biological profile. Mechanistic investigations revealed that PQM-250 disrupts mitochondrial function and redox homeostasis, processes essential for parasite survival. Treatment increased the production of reactive oxygen species, including hydrogen peroxide, and inhibited trypanothione reductase (TryR), impairing regeneration of the unique antioxidant defense system of trypanosomatids. This redox imbalance was accompanied by alterations in mitochondrial membrane potential, indicating mitochondrial dysfunction and events consistent with apoptosis-like cell death. Overall, PQM-250 induces redox collapse and mitochondrial dysfunction, emerging as a promising prototype for new pentamidine-derived leishmanicidal agents.

Pyrazole-nitroimidazole hybrids as promising anti-trichomonas agents

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Palavras Chave:*pyrazole,nitroimidazole,organic synthesis,chemotherapy,trichomoniasis*

Highlights

Pyrazole-nitroimidazole hybrids exhibited potent activity against*Trichomonas vaginalis*, the agent responsible fortrichomoniasis, the most important infection sexually transmitted (IST).

Resumo/Abstract

Imidazole derivatives, especially nitroimidazoles, have been widely evaluated against several protozoans. Two remarkable examples are metronidazole (MTZ) and tinidazole, drugs for the treatment of trichomoniasis, which showed many side effects. Therefore, the search for new candidates against Trichomonas vaginalis, the agent that cause trichomoniasis, is extremely relevant. Our research group has synthesized and evaluated the biological activity of several compounds containing heterocycle scaffolds. In this work, 10 2-(4-nitro-1*H*-imidazol-1-yl)ethyl 1-aryl-1*H*-pyrazole-4-carboxylates derivatives were synthesized in five steps, in 14-61% yields. The compounds were characterized by Fourier-transform Infrared (FT-IR) and Nuclear Magnetic Resonance (NMR) spectroscopies, and High-resolution Mass Spectrometry (HRMS). In FT-IR analyses, bands of stretchings related to C=O, C-H and nitro group were identified. The results of NMR analyses showed that all signals correspond to proposed structures. HRMS spectrum displayed*m/z*ratio $[M+Na]^+$ matching with the theoretical values, in errors ranging from 0.0 to 5.5 ppm. Regarding biological activity, all compounds showed high trichomonacidal activity (IC_{50} < 20 μM), highlighting 3 derivatives which IC_{50} values were 5.0 μM, very close to MTZ (IC_{50} = 4.9 μM), the reference drug. The cytotoxicity effect was also investigated against HeLa cells, which CC_{50} values were higher than 100 μM, except for one compound (CC_{50}= 69.3 μM). Among 10 derivatives assayed, 9 exhibited selectivity index (IS) higher than 10.

Agradecimentos/Acknowledgments

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Relationship between biomolecule interaction and cytotoxicity of photosensitizers in breast cancer cells during photodynamic therapy

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Palavras Chave:*Photodynamic therapy,Photosensitizer,Cytotoxicity,Breast cancer*

Highlights

PDT, allows cancer treatment, uses PS its mechanism. When excited by light, these PS cause cell death; but greater interaction of these substances with cells does not equate to greater cytotoxicity.

Resumo/Abstract

Photodynamic therapy (PDT) is a minimally invasive cancer treatment modality that relies on the generation of reactive oxygen species (ROS) by photosensitizers (PS) after irradiation with light of an appropriate wavelength. The interaction of PS with biomolecules is known as a critical factor that modulates photoinduced damage and determines the efficiency of cell death. This work aimed to investigate the relationship between the interaction with biomolecules and the cytotoxicity of two widely used PS, methylene blue (MB) and zinc phthalocyanine (ZnPc), in breast cancer cell models. The interaction of PS with biomolecules was evaluated by quantifying their association with proteins, lipids, and DNA, and cellular uptake was determined in MDA-MB-231 cells, a triple-negative breast cancer model. ZnPc showed greater interaction with biomolecules and greater cellular uptake in MDA-MB-231 cells compared to AM, both at the same concentration of 10 µM and with varying incubation times (2h, 4h, 6h, and 24h). However, cytotoxicity and phototoxicity assays performed on MDA-MB-231 and MCF-7 cells, under different concentrations (0.10-10 µM) and irradiation doses (0–6 J/cm²) varied by different irradiation times (0, 11, 22, and 32 min), revealed that MB induced more pronounced oxidative damage, reducing cell viability at lower concentrations than ZnPc. These findings indicate that a stronger interaction of a photosensitizer with biomolecules and cells does not necessarily translate into greater photoinduced damage, questioning the assumption that greater absorption invariably leads to greater efficacy of photodynamic therapy (PDT). The observed differences may be associated with a greater contribution of type I mechanisms and the greater aqueous solubility of MB, a hypothesis that is being investigated in ongoing experiments.

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Research aiming at identification of cinnamoyl-N-hydrazones with antiviral activity against orthopoxviruses.

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Palavras Chave:*Monkeypox,Antiviral activity,Vaccinia virus,Orthopoxvirus,Zoonotic disease*

Highlights

Initial screening of hybrid compounds reveals two promising antiviral candidates against Orthopoxvirus.

Resumo/Abstract

The Monkeypox virus (MPV), the etiological agent of monkeypox, is a zoonotic virus identified in 1958, with the first human infection recorded in 1970 in the Democratic Republic of the Congo. Recently, it was re-emerged as a public health emergency of international concern by the World Health Organization (WHO) in 2022 and again in 2024. MPV transmission occurs between animals, from animals to humans and between humans. Currently, treatment is based on symptomatic management, as chemotherapeutic alternatives or specific vaccines are still lacking; smallpox vaccines are used due to cross-protection. In this context, we investigated a series of twelve cinnamoyl-N-acyl-hydrazones derivatives, using the Vaccinia virus (VACV) as a preliminary experimental model to evaluate antiviral activity. Assays were performed in duplicate using BSC-40 cells, infected with 80 plaque-forming units (PFU) and treated with compounds at 100µM. Three compounds showed evident citotoxicity, while two stood out by reducing the viral load by over 95%. Given these preliminary results, other research is in progress, including in vivo bioavailability studies, aiming for better pharmacological characterization and an intellectual property protection at the Instituto Nacional de Propriedade Intelectual (INPI).

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Agradecimentos/Acknowledgments

49 Anual Meeting of the Brazilian Chemical Society, PeQuiM - Medicinal Chemistry Research Laboratory; INCT-Inofar; FAPEMIG, CAPES, CNPq, Finep, Unifal-MG.

Se-functionalized pyrazoles with potential antiviral activity against ZIKV and MAYV

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Palavras Chave:*Heterocycles, selenium, ZIKV, MAYV, functionalization*

Highlights

This work reports the biological evaluation of pyrazole–selenium derivatives identifying lead compounds with ≥90% dual inhibition against ZIKV and MAYV.

Resumo/Abstract

Arboviruses such as Zika (ZIKV) and Mayaro (MAYV) have become increasingly relevant public health threats, especially due to the absence of approved antiviral therapies[1]. Consequently, the search for new bioactive molecules is highly necessary, and the association of pyrazoles with selenium, given their known biological activities[2] represents a promising strategy. In this context, and inspired by a recently described one-pot selenium functionalization of pyrazoles[3], the present work investigates the antiviral activity of these compounds against ZIKV and MAYV. Using this approach, a library of 21 derivatives was assessed for antiviral activity (Figure 1). Among the evaluated molecules, compounds**1h**and**1o**demonstrated pronounced dual inhibitory effects against both ZIKV and MAYV (≥90%) while maintaining low cytotoxicity (CC_{50} > 360 µM), identifying them as the most promising candidates. Although compounds**1d**and**1e**also showed significant antiviral activity, their lower CC_{50} values (269 µM and 209 µM, respectively) suggest increased cytotoxicity. Consequently, compounds**1h**and**1o**emerged as lead candidates, combining strong dual antiviral activity against ZIKV and MAYV with low cytotoxicity, which supports their further investigation as potential antiviral agents.

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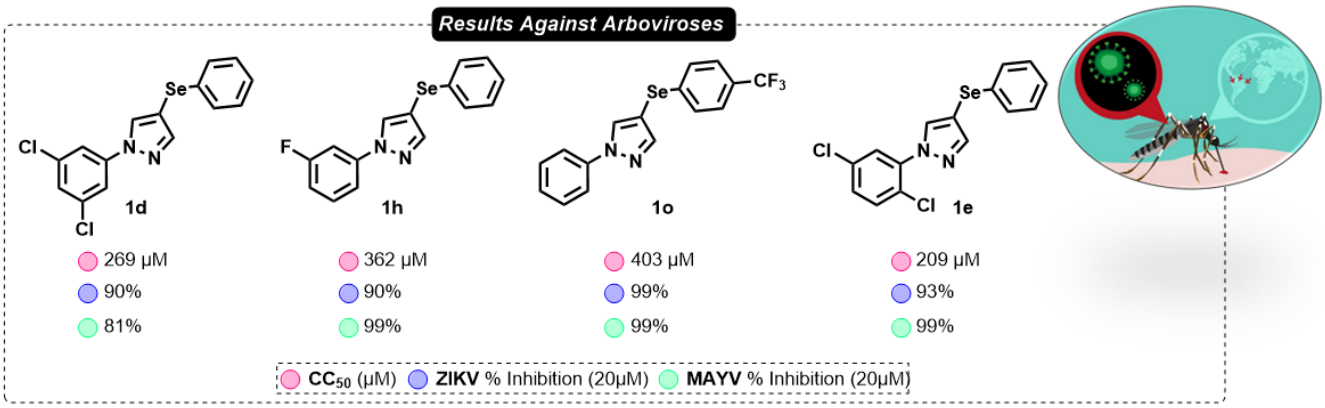


Figure 1. Activity of 4-selanylpyrazoles against Arboviruses.

Agradecimentos/Acknowledgments

UFF, CNPq, CAPES, FAPERJ.

STRUCTURAL OPTIMIZATION AND BIOLOGICAL EVALUATION OF N-BENZYL PURINE–BENZOHYDROXAMATE HYBRIDS AS DUAL JAK3/HDAC6 INHIBITORS FOR THE TREATMENT OF HEMAT

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Palavras Chave:*Hybrid inhibitors, bioisosterism, HDAC6, JAK3, hematologic malignancies,Hybrid inhibitors,bioisosterism,HDAC6,JAK3,hematologic malignancies*

Highlights

Dual JAK3/HDAC6 hybrids with potent anticancer activity were identified.**6b**and**6f**show submicromolar activity in leukemia/lymphoma cells. All compounds are highly selective HDAC6 inhibitors (IC_{50} < 1 nM).**6f**shows low toxicity in normal cells

Resumo/Abstract

The enzymes JAK3 and HDAC6 are relevant therapeutic targets in hematologic malignancies due to their roles in cytokine signaling and proteostasis. Aberrant JAK3 activation and HDAC6 activity contribute to tumor progression and therapeutic resistance. Therefore, dual targeting of JAK3 and HDAC6 represents a rational strategy to enhance therapeutic efficacy. In this context, N-benzil-purine–benzohydroxamate hybrids were designed and synthesized as two series of compounds (**series 1**and**2**), starting from the promising lead compound**6a**, and incorporating pharmacophoric features compatible with JAK3 inhibition and selective HDAC6 chelation (**Figure 1A**). A three-step synthetic route (**Figure 1B**) afforded eight final compounds (**6a–h**) with overall yields of 25–37% and high purity (95.3–99.4%), enabling preliminary structure-activity relationship analysis. Compounds**6b**and**6f**emerged as the most potent derivatives, displaying submicromolar antiproliferative activity in leukemia and lymphoma cell lines (Jurkat, Namalwa, SET2, and U937) and outperforming ruxolitinib in several models. The entire series showed extremely potent HDAC6 inhibition (IC_{50} < 1 nM), while HDAC1 inhibition remained in the micromolar range, indicating pronounced selectivity for HDAC6. Moderate inhibition of HDAC8 further supports a predominantly HDAC6-selective profile (**Figure 1C**). Compound**6f**combined high cellular potency with reduced cytotoxicity in non-tumoral colon and skin cells, suggesting preliminary tumor selectivity. A clear stereochemical effect was observed, with**6b**(*R*) being more active than its enantiomer**6c**. Compound**6d**showed moderate activity with preference for hematologic cells, while**6e**displayed lineage-dependent effects (**Figure 1C**). Overall,**6b**and**6f**emerge as promising lead candidates for dual JAK3/HDAC6 inhibitors for hematologic malignancies, combining high cellular potency, strong and selective HDAC6 inhibition, and encouraging preliminary safety. Future studies will include enzymatic assays against JAK3 and mechanistic analyses to confirm dual-target engagement and support further optimization.

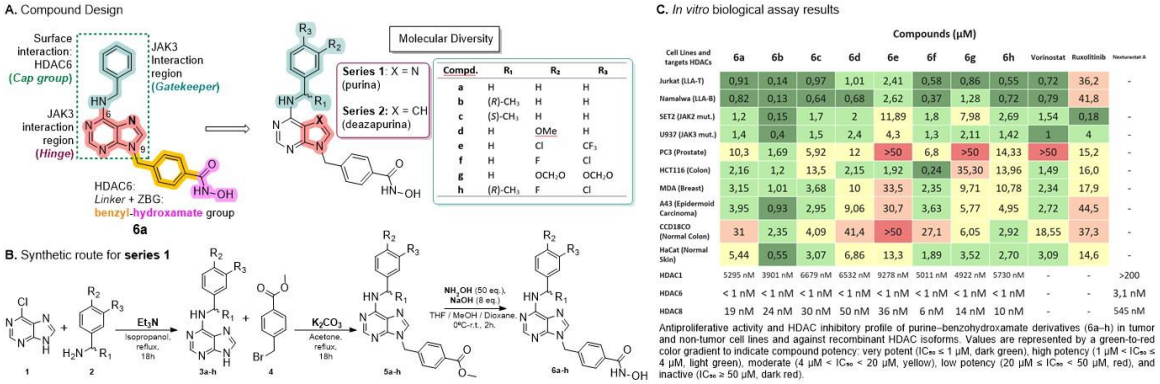


Figure 1: A) Compound Design; B) Synthetic route for series 1; C) In vitro biological assay results

Agradecimentos/Acknowledgments

The authors are grateful to Faculty of Pharmacy of University of São Paulo, which allowed the development of this work #2024/07723-2 from FAPESP.

Structure-Based Design of Dual PDE3/PDE4 Modulators Derived from the LASSBio-1632 Scaffold

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Palavras Chave:*SBDD, LBDD, PDE3, Sulfonylhydrazone, Molecular Docking,SBDD,LBDD,PDE3,Sulfonylhydrazone,Molecular Docking*

Highlights

Structure-based analysis of PDE3A and PDE3B binding modes

Docking-guided optimization of LASSBio-1632 prototype

Identification of key interaction gaps within the PDE3 catalytic pocket

Resumo/Abstract

Phosphodiesterases (PDEs) are zinc- and magnesium-dependent metalloenzymes that regulate cyclic nucleotide signaling and play pivotal roles in inflammatory responses and bronchial smooth muscle tone. In chronic obstructive pulmonary disease (COPD), PDE4 inhibition is clinically validated, while increasing evidence suggests that concomitant modulation of PDE3 may further improve therapeutic outcomes through bronchodilation and smooth vascular muscle relaxation. Within this context, LASSBio® has previously developed compound 1, an optimized analogue of LASSBio-1632 lead-compound, which displays low-nanomolar potency toward PDE4 isoforms, reduced blood–brain barrier permeability, and partial inhibition of PDE3A, motivating a structure-based investigation of its molecular recognition profile.

In this study, molecular docking studies were conducted using PDE3A (PDB ID: 7L28) and PDE3B (PDB ID: 8SYC), employing trequinsin and GSK4394835A as reference ligands. Redocking validation identified the CHEMPLP scoring function as the most reliable, yielding RMSD values between 1.26 and 2.03 Å. Binding mode analysis revealed conserved hydrogen-bond interactions with Ser1003 in PDE3A and Asn830 and His737 in PDE3B, π–π stacking with phenylalanine residues, and a favorable orientation of the sulfone moiety toward the Mg^{2+} catalytic site. Nonetheless, key interaction hotspots involving Gly940, Ile955, Tyr736, and Phe939 were not fully exploited by the parent scaffold.

Based on these structure-based insights, five new LASSBio-1632 analogues were rationally designed to enhance molecular complementarity and recover critical interactions within the PDE3 catalytic pocket. Ongoing studies include comparative docking using multiple platforms and ensemble-based pharmacophore modeling, aiming to support the development of dual PDE3/PDE4 modulators as promising candidates for COPD therapy.

Agradecimentos/Acknowledgments

Authors would like to thank FAPERJ, INCT-INOFAR, CAPES and CNPq for financial support.

Studies Towards the Identification of New Triazole-Based Multitarget Anti-SARS-CoV-2 Drug Candidate Prototypes: The Discovery of PQM-262

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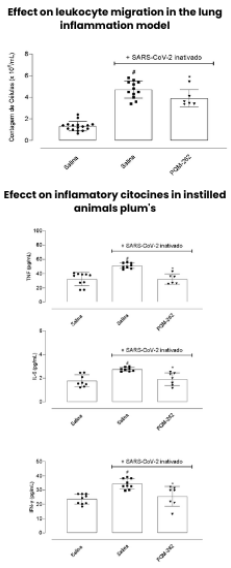
Palavras Chave:*SARS-CoV-2,Antiviral,COVID-19,Hidrazones,Triazole derivatives*

Highlights

PQM-262 showed potent multitarget activity against SARS-CoV-2.
A repositioned triazole–hydrazone hybrid emerged as a novel anti-COVID-19 candidate.

Resumo/Abstract

The SARS-CoV-2 virus causes severe pneumonia, which can progress to multiple organ failure and death, especially in patients with comorbidities. This virus has high transmissibility, being spread through respiratory microdroplets from infected patients. Even with pharmaceutical approaches, such as Paxlovid, the emergence of new variants still makes the search for new strategies to combat this virus a global priority, being of high cost to the public health services [3]. In this context, hydrazides and hydrazones-derived compounds have shown to be promising drug candidates, especially when combined with triazole rings, known for their antimicrobial potential [1, 2]. This work addresses a new use for the triazole-hydrazone hybrid PQM-262, which was originally designed as a leishmanicidal agent. However, due to the pandemic emergency and international engagement to discover new chemical entities against SARS-CoV-2, a repositioning screening was performed with a series of triazole analogues from our chemical library. As a result, PQM-262 was identified as a potent SARS-COV-2 inhibitor and was then selected for further pharmacological studies. In vitro and in vivo results stood out the multitarget antiviral activity profile of this compound, acting as a significant virus replication suppressor (IC50= 0.064 μM), ACE-2 antagonist (IC50= 12.7 nM), being more potent than the standard antagonist DX600 (8.56 μM), and anti-inflammatory in in vivo pneumonia models, reducing TNF alpha, IL-6, and IFN-γ and the leukocyte migration (Image). Overall, these experimental data highlight PQM-262 as an innovation, with a higher potential therapeutic character than other approved anti-COVID-19 drugs, leading to a patent deposit (BR 1020240229410).
[1]https://doi.org/10.3390/vaccines9091012
[2]https://doi.org/10.1038/s41586-020-2577-1
[3] https://doi.org/10.1038/s41598-024-76472-0



Effect of PQM-262 in leukocyte migration and on cytokines reduction.

Agradecimentos/Acknowledgments

The authors are grateful to CNPq, FAPEMIG, FAPERJ, CAPES, FINEP, and INCT-INOFAR for financial support and fellowships.

Synthesis and Antifungal Activity of 4-Arylamino-1,2-naphthoquinone-1,2,3-triazole Hybrids

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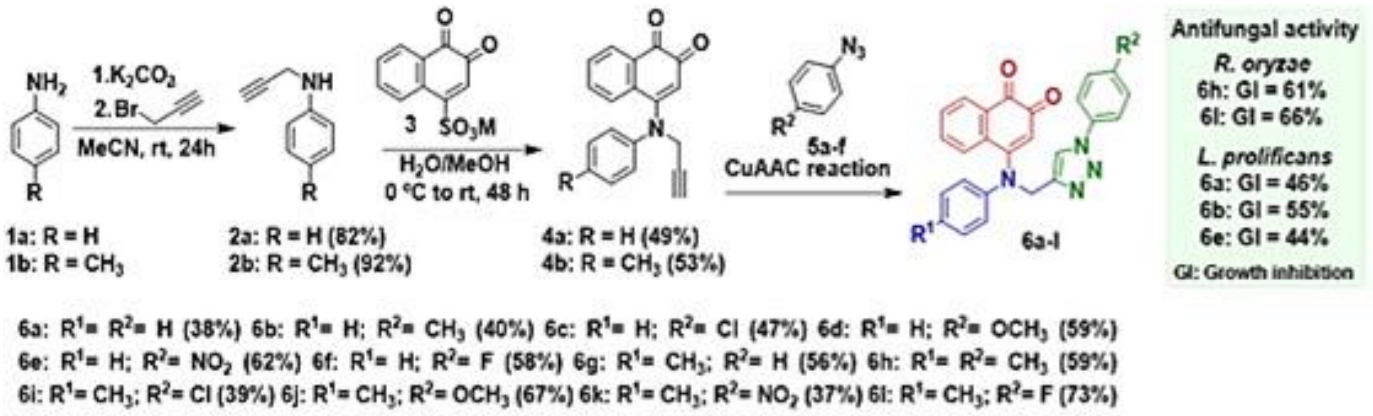
Palavras Chave:*Quinone, Triazole, Molecular hybridation, Candida spp,Quinone,Triazole,Molecular hibridization,Candida spp*

Highlights

Synthesis of novel naphthoquinone-triazole derivatives with antifungal activity against drug-resistant species. Except for**6g**, all the compounds presented antifungal activity in the 107 - 123 μM range.

Resumo/Abstract

Quinones have been strategically combined with various heterocyclic scaffolds to enhance their biological properties. In this work, a new series of hybrid 1,2-naphthoquinone derivatives bearing a 1,2,3-triazole ring was synthesized via an efficient multistep procedure. The first stage involved alkylation of commercial anilines**1a**and**1b**with propargyl bromide, affording**2a**and**2b**in 82% and 92% yields, respectively. In the second step, nucleophilic substitution between 1,2-naphthoquinone salt**3**and anilines**2a-b**produced type**4**alkynes in yields of 49% and 53%, respectively. In the third step, the naphthoquinone-triazole hybrid type**6**was synthesized via Cu(I)-catalyzed azide–alkyne cycloaddition (CuAAC) of aryl azides**5**with terminal alkynes of type**4**. The hybrids**6a-l**were obtained in yields of 37% to 73%. Biological evaluation revealed that most compounds exhibited antifungal activity, particularly against*Lomentospora prolificans*and*Rhizopus oryzae*, which are often resistant to conventional antifungal drugs. Notably, this activity was not mediated by ROS generation and did not involve inhibition of lanosterol 14α-demethylase (CYP51), suggesting an alternative mechanism of action. Structure–activity relationship analysis indicated that both R^1 and R^2 substituents play a significant role in modulating antifungal activity, although their effects varied across fungal species. Overall, the structural diversity of these novel 1,2-naphthoquinone-1,2,3-triazole hybrids enables a range of molecular interactions with fungal targets, making them promising candidates for developing novel antifungal agents, particularly given the high prevalence of fungal infections in human colonization and their clinical significance.



Synthesis of novel antifungal 4-arylamino-1,2-naphthoquinone-triazole hybrids

Agradecimentos/Acknowledgments

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Synthesis and Antileishmanial Activity of Chalcones from Dracaena cinnabari

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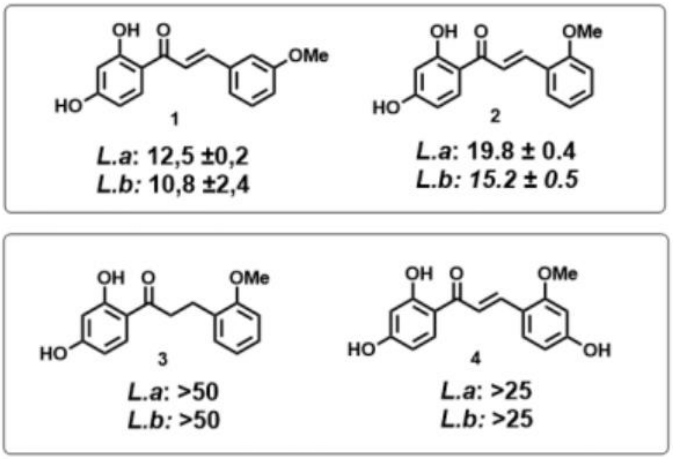
Palavras Chave:*chalcones,Leishmaniasis,Leishmania*

Highlights

Four chalcones from*D.cinnabari*were designd and synthesized. The most active compond 1, showed EC_{50} values of 12.5 µM and 10.8 µM against*L. amazonensis*and*L. braziliensis.*

Resumo/Abstract

Four chalcones were synthetized in 3–4 steps with overall yields ranging from 13% to 19%. Their structures were confirmed by ^1H and ^13C NMR spectral data analysis. 2',4'-Hydroxy-3-methoxychalcone (1) and 2',4'-hydroxy-2-methoxychalcone (2) were active against Leishmania amazonensis with EC50 values of 12.5 µM and 19.8 µM, respectively. Compounds 1 and 2 also displayed activity against Leishmania braziliensis, presenting EC50 values of 10.8 µM and 15.2 µM, respectively. These results are consistent with previous reports describing chalcones as promising scaffolds for the development of antileishmanial agents, mainly due to the presence of an α,β-unsaturated carbonyl system capable of acting as a Michael acceptor and interacting with nucleophilic targets in the parasite. Considering that leishmaniasis remains a neglected tropical disease and that the currently available treatments are limited by toxicity, high cost, and the emergence of resistant strains, the search for new antileishmanial compounds is of great importance. In this context, chalcones have attracted considerable attention because of their structural simplicity, synthetic accessibility, and broad spectrum of biological activities. Altogether, our results indicate that chalcones isolated from Dracaena cinnabari represent promising candidates for further investigation as potential antileishmanial agents.



Chalcones derived from D. cinnabari and their leishmanicidal activities.

Agradecimentos/Acknowledgments

The authors acknowledge financial supports from CAPES, CNPq and FAPESP.

Synthesis and Antimicrobial Evaluation of Nimesulide Triazole Derivatives Guided by Target Fishing

Alessandro Kappel Jordão (PQ)*[1], Antônio Carlos Alexandre da Silva (PG)[1], Deysiane Oliveira Brandão (PQ)[1], Rita Yanka Pereira da Silva (PG)[1], Lamark Carlos I (PG)[1], Euzébio Guimarães Barbosa (PQ)[1].

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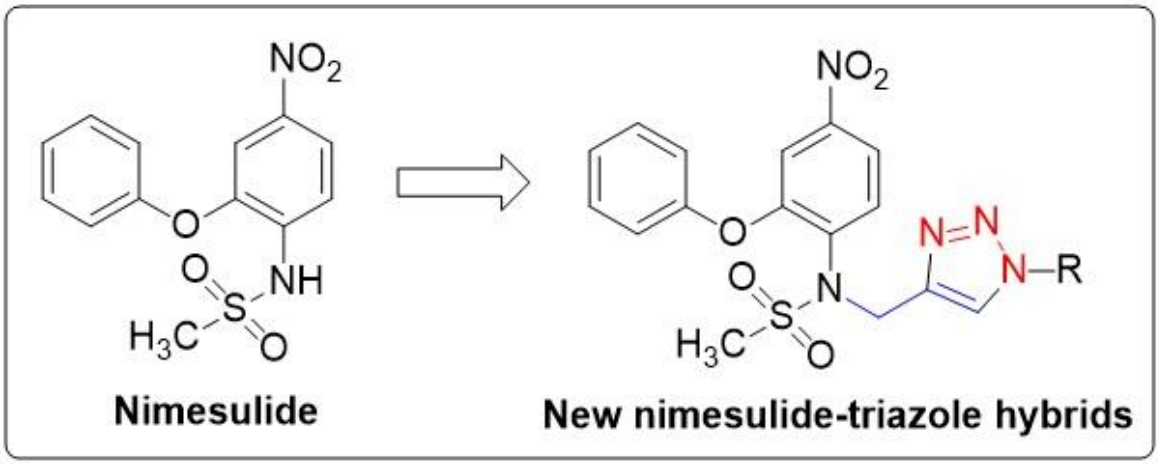
Palavras Chave:*Nimesulide,Triazoles,Antimicrobial Evaluation,Synthesis,Target Fishing*

Highlights

Synthesis of novel triazole derivatives based on nimesulide; New compounds obtained in good overall yields; Compounds showed antimicrobial activity against Gram-positive and Gram-negative bacteria

Resumo/Abstract

Antimicrobial resistance (AMR) poses a serious and growing threat to global health, prompting the World Health Organization to emphasize the urgent need for new agents active against multidrug-resistant pathogens. Recent studies identify AMR as a leading cause of death worldwide, with millions of deaths already associated with resistant infections and projections indicating a substantial increase by 2050.[1] The most significant contributors to AMR-related mortality include*Escherichia coli*,*Staphylococcus aureus*, and*Klebsiella pneumoniae*, underscoring the critical magnitude of this challenge. In this context, the search for new therapeutic strategies includes the repositioning and modification of existing drugs.[2] This work describes the synthesis, characterization, and biological evaluation of a novel series of 1*H*-1,2,3-triazole-1,4-disubstituted compounds derived from nimesulide. Eleven new compounds were synthesized, including one terminal acetylene intermediate and ten triazole derivatives, with overall yields considered good (75–92%). Structural characterization was carried out using spectroscopic techniques, including infrared (IR) spectroscopy and ^{1}H and ^{13}C nuclear magnetic resonance (NMR), confirming the proposed structures. In addition, the antimicrobial activity of the synthesized compounds was investigated against*Staphylococcus aureus*,*Escherichia coli*, and*Klebsiella pneumoniae*. A target fishing approach was employed to predict potential biological targets and to further evaluate the antimicrobial activity of the most promising compounds, both alone and in combination with commercial antibiotics, against the same bacterial strains. Preliminary results indicate that these new nimesulide–triazole hybrids show potential for the development of novel antimicrobial agents.
[1] Okwu, M. U.*et al.*,*AIMS Microbiol.*2019,*5*, 117. [2] Niu, D.*et al.*,*Pattern Recognit.*2026,*171*, 112114



Nimesulide-triazole hybrids

Synthesis and Cytotoxic Activity of 2-Styrylbenzothiazole and 2-Styrylbenzimidazole Derivatives: Insights from DNA/BSA Binding and Molecular Docking

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Palavras Chave:*2-styrylbenzothiazoles; 2-styrylbenzimidazoles; organic synthesis; sodium bisulfite-mediated reaction; anticancer activity*

Highlights

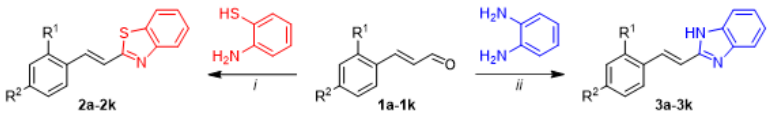
significant biological potential

Resumo/Abstract

Malignant breast neoplasia is the most prevalent type of cancer among women, with more than 2 million new cases diagnosed annually. Given its high incidence and the elevated mortality rates associated with this disease, the search for new effective therapeutic agents has been intensified. In this context, heterocyclic compounds such as benzothiazoles and benzimidazoles have attracted considerable attention due to their pronounced cytotoxic activity against different tumor cell lines, emerging as promising anticancer agents[1]. The synthetic routes traditionally employed for the preparation of these compounds generally involve harsh conditions, such as strongly acidic environments and elevated temperatures. In this study, we report the microwave-assisted synthesis of a series of styrylbenzothiazoles and styrylbenzimidazoles in the presence of sodium bisulfite ($NaHSO_3$)[2], along with the evaluation of their cytotoxic activities against the tumor cell lines MDA-MB-231 and 4T1, using MCF-10A cells to assess selectivity. Compound 2f, an amino-substituted derivative, exhibited the highest cytotoxic activity (IC_{50} = 4.0 μM), being twice as potent as the reference drug cisplatin (IC_{50} = 9.6 μM) and 9- to 25-fold more potent than the other derivatives in the series. Styrylbenzimidazole derivatives 3d, 3g, and 3k also showed promising activity against MDA-MB-231 cells, with IC_{50} values of 8.2, 6.6, and 5.9 μM, respectively. Competitive DNA binding studies involving compounds 2d, 2f, 3d, and 3f with ethidium bromide (EB) or 4′,6-diamidino-2-phenylindole (DAPI) suggested a preferential interaction with DNA through the minor groove, while interaction assays with bovine serum albumin (BSA) confirmed their protein-binding ability. These results were further supported by molecular docking and DFT calculations.

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2-styrylbenzothiazoles	R^1	R^2	Yield (%)	2-styrylbenzimidazoles	R^1	R^2	Yield (%)
2a	H	H	67	**3a**	H	H	82
2b	H	OCH_3	74	**3b**	H	OCH_3	88
2c	H	NO_2	58	**3c**	H	NO_2	34
2d	OCH_3	H	69	**3d**	OCH_3	H	73
2e	NO_2	H	54	**3e**	NO_2	H	59
2f	H	$N(CH_3)_2$	61	**3f**	H	$N(CH_3)_2$	99
2g	H	F	82	**3g**	H	F	74
2h	H	CN	57	**3h**	H	CN	52
2i	H	SCH_3	75	**3i**	H	SCH_3	64
2j	H	Br	83	**3j**	H	Br	49
2k	H	CF_3	55	**3k**	H	CF_3	61

Synthesis of 2-styrylbenzothiazole (BT) and 2-styrylbenzimidazole (BZI) derivatives.

Agradecimentos/Acknowledgments

CNPq, CAPES and FAPEMIG.

Synthesis and Zika NS2B–NS3- Protease Inhibitory Activity of a Chalcone from Dracaena cinnabari

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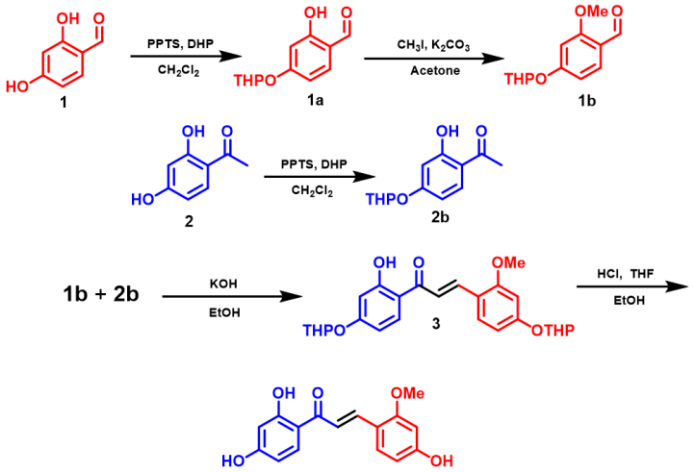
Palavras Chave:*Chalcones,NS2B-NS3 Protease,Zika Virus,Enzyme Inhibition,Chalcone*

Highlights

4,2',4'-Trihydroxy-2-methoxychalcone (**1**) is a major chalcone of*Dracaena cinnabari*
Compound**1**was synthesized with 10% overall yield.
Compound**1**inhibited Zika protease (IC_{50} = 41.1 µM).

Resumo/Abstract

This study describes the synthesis of a chalcone (ZIka) and the evaluation of inhibitory activity against the NS2B-NS3 protease of Zika virus. The synthetic route allowed the obtention of the target compound with an overall yield of 10% after five steps and chromatographic separations. The biological activity was investigated by*in vitro*enzymatic assays, in which the chalcone has significantly inhibited the viral protease activity, with an IC_{50}value of 41.1 µM. These findings indicate the compound represents a promising hit for the development of new NS2B-NS3 protease inhibitors, highlighting the relevance of chalcones as valuable compounds in antiviral drug discovery.



Synthetic route of 4,2',4'-trihydroxy-2-methoxychalcone from Dracaena cinnabari

Agradecimentos/Acknowledgments

CAPES, CNPq and FAPESP.

Synthesis, Characterization, and Structural Evaluation of New Quinazolinone Derivatives with Pharmacological Potential

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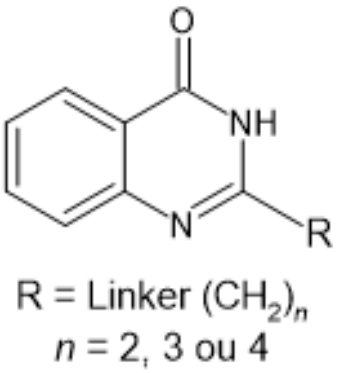
Palavras Chave:*Quinazolinones,NMR spectroscopy,Organic synthesis,Antimicrobials,Medicinal chemistry*

Highlights

Quinazolinone derivatives represent a strategic scaffold in Medicinal Chemistry for the development of new bioactive molecules.

Resumo/Abstract

The increasing incidence of multidrug-resistant bacteria has promoted the search for new bioactive molecules, reinforcing the importance of rational molecular design in the development of therapeutically relevant compounds. In this context, quinazolin-4(3H)-ones (Figure 1) are recognized as a privileged scaffold in Medicinal Chemistry, widely investigated due to their structural versatility and reported antimicrobial properties. This work reports the synthesis and characterization of a novel series of quinazolin-4(3H)-one derivatives, rationally designed through targeted structural modifications to expand the chemical space of this class and generate new candidates with potential pharmacological applications. The compounds were synthesized via a convergent six-step route using anthranilamide as the precursor. Purification was achieved by solid-phase extraction (SPE), employing a gradient of acetonitrile (15–100%) in 20 mM ammonium acetate solution, which proved to be an effective and scalable approach for isolating the desired products. Structural elucidation and purity assessment were performed by one- and two-dimensional NMR (^{1}H, ^{13}C, COSY, HSQC, and HMBC) and LC–MS analyses, supported by the infrastructure of the Brazilian Biosciences Laboratory (LNBio/CNPEM). The developed methodology enabled the synthesis of four new quinazolin-4(3H)-one derivatives, designated JSSA, with average isolated yields of approximately 70%. All compounds exhibited high chemical purity, exceeding 95%. Based on these results, the newly synthesized compounds will be subjected to biological evaluation to assess their antimicrobial potential. In parallel, additional analogs stemming from the rational expansion of this series are currently in advanced stages of synthesis and purification, aiming to further explore structure–activity relationships and support future pharmacological studies.



Quinazolinone structure with an R substituent corresponding to a variable-length carbon linker.

Agradecimentos/Acknowledgments

We thank our collaborators, the School of Pharmaceutical Sciences at Unicamp, the Brazilian Biosciences Laboratory (CNPEM), the Ministry of Science, Technology and Innovation, FAPESP (2024/11146-0), and CNPq (132492/2024-5).

Synthesis, in vitro and in vivo antitumoral effect against OSCC of new dithioethers based on catalyst-free Michael addition of thiols to α-xyloidone

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Palavras Chave:*pyranonaphthoquinones,thia-Michael addition,oral cavity cancer,apoptosis celular*

Highlights

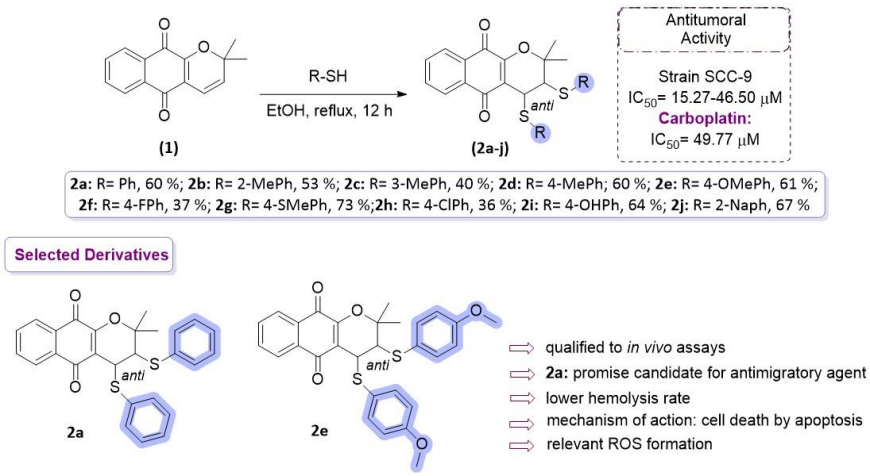
Ten new dithioethers. Two derivatives qualified for in vivo trials: promising candidates as anti-migration agents, low hemolysis rate, apoptotic mechanism of action, and significant ROS formation.

Resumo/Abstract

Oral squamous cell carcinoma is the most common malignant tumor of the oral cavity, with ~390,000 new cases and 188,000 deaths worldwide. From a synthetic standpoint, pyranonaphthoquinones are natural compounds widely studied for their biological activities, especially xyloidones and lapachones. However, functionalization of the pyran ring mainly relies on lapachones, while xyloidones remain underexplored and typically require additional steps. Thus, this work aims to synthesize new thioethers through direct functionalization of α-xyloidone and evaluate their antitumor activity. The Michael addition of thiols to α-xyloidone**(1)**led to the formation of ten dithioethers**(2a-j)**with yields between 36-73%. An initial screening against human tongue squamous cell carcinoma (SCC-9) showed an IC_{50} range between 15.27 and 46.50 μM (reference: carboplatin, IC_{50}= 49.77 μM). Dithioethers**2a**and**2e**, qualified in initial tests after evaluation in three different oral squamous cell carcinoma strains, were able to inhibit SCC-9 cell migration by 71.7 and 45.3%, respectively.**2a**showed a promise candidate for antimigratory agent, indicating a lower risk of metastatic cancer. In hemolysis assays,**2a**presented a rate of 1.06%, lower than carboplatin (1.34%). The mechanism of action of these dithioethers showed an induction of cell death by apoptosis and significant formation of reactive oxygen species. The relevant results show the potential of this molecules, obtained in this work in a single step from α-xyloidone for the first time in the literature [1-3].

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[2] Washwa, P.; Kharbanda, A.; Sharma, A.*Asian J. Org. Chem.***2018**, 7, 634-661.
[3] Lee, Y.; Choi, J.; Trinh, D.; Kim, N.*Synthesis***2005**, 18, 3026-3034.



Synthesis of dithioethers (2a-i) and promising derivatives

Agradecimentos/Acknowledgments

PPGQ-UFF, CAPES, FAPERJ, CNPq

Synthesis of Caffeine Derivatives and Evaluation of Their Anticholinesterase Activities

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Palavras Chave:*Acetylcholinesterase inhibitors,Caffeine,Semi-synthesis,Ethers,Molecular docking*

Highlights

Semi-synthesis of caffeine derivatives; biological assays for the evaluation of anti-acetylcholinesterase activity; molecular docking studies.

Resumo/Abstract

The significant medicinal and agrochemical potential of cholinesterase inhibitors has driven continued interest in discovering novel molecules, particularly those with distinct structural scaffolds. In this context, caffeine was selected as the core scaffold for the design of new anticholinesterase agents, owing to its neuroprotective effects and favorable blood–brain barrier permeability, which facilitates central nervous system activity. In this study, six caffeine derivatives were synthesized with yields ranging from 51% to 95%, incorporating functional groups inspired by commercially available acetylcholinesterase (AChE) inhibitors. Notably, the brominated derivative exhibited the highest inhibitory activity, achieving 55% inhibition at 50 μmol L^{-1}. Computational investigations indicate that its formation likely proceeds via an electrophilic aromatic substitution (SEAr) mechanism rather than a radical pathway. Moreover, molecular docking analyses and physicochemical evaluations reveal that reduced molecular volume is associated with enhanced AChE inhibitory potency. Although the inhibition percentage is lower than that of the positive control (galantamine), this structure appears promising as it represents a novel structural scaffold with anti-AChE activity. This characteristic is relevant both in the context of acquired resistance to agrochemicals acting via this mechanism and in the development of new anti-AChE drug candidates.

Agradecimentos/Acknowledgments

CAPES; CNPq; FAPEMIG; FINE; EMBRAPA-Café; INCT-Defesa.

Synthesis of chalcone analogues with conformational restriction potentially antimycobacterial

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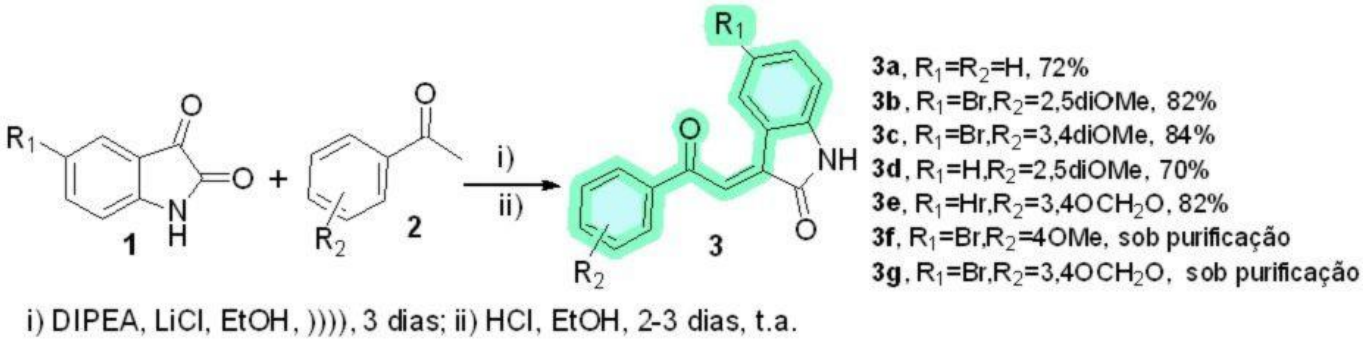
Palavras Chave:*Chalcona,Aldol,Restrição Conformacional,Tuberculose*

Highlights

In this work we describe the synthesis of aldol adducts that were dehydrated to obtain conformationally restricted chalcone analogs. Our group will test their antimycobacterial activity.

Resumo/Abstract

As chalconas são cetonas aromáticas α,β-insaturadas que representam uma classe de moléculas de grande interesse para a pesquisa científica devido à sua diversidade de ações biológicas Ensaios*in vitro*e *in vivo*têm demonstrado que as chalconas possuem atividades anti-inflamatória, anticâncer, neuroprotetora e antimicobacteriana. Pesquisas corroboram a capacidade das chalconas e seus derivados em inibir o crescimento de*Mycobacterium tuberculosis*(Mtb), incluindo cepas resistentes aos fármacos de primeira linha. O presente trabalho tem como objetivo a síntese de análogos de chalconas com restrição conformacional, denominados híbridos chalcona-isatina, visando à avaliação de sua atividade antimicobacteriana. Inicialmente, a reação de aldol foi conduzida entre diferentes metil-cetonas e isatina, uma cetona desprovida de hidrogênios alfa, utilizando etanol e THF como solventes, na presença de bases orgânicas e inorgânicas (como DBN, DIPEA e KOH). As tentativas de reprodução de protocolos descritos na literatura revelaram-se ineficazes para este sistema específico, envolvendo duas cetonas aromáticas de baixa reatividade, resultando na ausência do produto desejado ou exigindo tempos reacionais excessivamente longos (8 dias). As condições reacionais foram otimizadas mediante o uso de ultrassom e cloreto de lítio como catalisador, mantendo a temperatura entre 30 e 40 ºC. Por meio deste método, foram obtidos sete produtos da reação aldólica, com rendimentos variando entre 34% e 65%. A subsequente desidratação desses intermediários, utilizando HCl e etanol, forneceu 7 análogos de chalcona com bons rendimentos (70% a 82%), duas das quais estão sendo purificadas. As chalconas estão sendo submetidas a ensaios de atividade antimicobacteriana pelo nosso grupo de pesquisa, cujos resultados serão apresentados no evento. A síntese de outros análogos de chalcona está em andamento.



Formação dos análogos de chalcona.

Agradecimentos/Acknowledgments

À Farmanguinhos pelas análises e à FAPERJ pelo auxílio financeiro para a pesquisa.

Synthesis of new 1,2,3-triazole compounds exhibiting anticancer activity

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Palavras Chave:*123-triazole,Organic synthesis,Bioactivity,Anticancer*

Highlights

Synthesis of new 1,2,3-triazole compounds; 1,3-dipolar cycloaddition click reaction; Biological assay against the MCF-7 and SK-MEL-147 human cancer lineages.

Resumo/Abstract

The 1,2,3-triazole is a synthetic heterocycle that is of great interest in the research of new bioactive compounds. This is due to its variety of biological activities, such as anticancer, and its use as a linker in molecular hybridization. Although chemotherapy is still the most common treatment for cancer, it poses the problem of drug resistance, which is the cause of approximately 90% of cancer mortality. This makes the search for new compounds that inhibit proliferative activity while causing less resistance fundamental, especially since cancer is the second largest cause of death worldwide. With this in mind, new organic molecules containing the 1,2,3-triazole heterocycle and pyridine scaffolds were synthed and their inhibitory potential was tested against cancerous cells. Twenty new pyridinyl 1,2,3-triazole derivatives were obtained in a 1,3-dipolar cycloaddition click reaction catalyzed by copper(I) (CuAAC), involving an azide and functionalized terminal alkynes containing donating and withdrawing groups on the aromatic ring (OCH3, CH3, F, Cl, Br, I). The compounds, which had yields between 53 and 95%, were characterized with spectroscopic and spectrometric techniques. The biological assay was done against the MCF-7 (estrogen receptor-positive breast cancer) and SK-MEL-147 (melanoma) human cancer lineages, and cellular viability was determined via a Sulforhodamine B (SRB) assay. Most compounds didn't significantly reduce cellular viability on the lineages tested, however GT14 and GT19 showed promising results. GT14 reduced cellular viability for MCF-7 by around 50%, while GT19 reduced cellular viability for SK-MEL-147 by approximately 50%. As such, these studies point to molecular enhancement through the synthesis of more potent analogues against tumour cells by analysing which molecules perform better and basing future research on modifying them.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPEMIG, FINEP, EMBRAPA-Café and INCT-Defesa.

Theoretical Determination of Binding Modes for GSK-3β-Targeting PROTACs in Alzheimer's Disease

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Palavras Chave:*Alzheimer´s Disease, PROTAC, Drug Discovery, Molecular Modeling*

Highlights

GSK-3β is a key target in Alzheimer's disease;

PROTACs enable selective protein degradation;

Ternary complex formation drives PROTAC efficiency;

Molecular modeling supports PROTAC design.

Resumo/Abstract

Alzheimer's disease (AD) is a neurodegenerative disorder for which no disease-modifying therapies are currently available. Glycogen synthase kinase-3 beta (GSK-3β) plays a central role in the molecular mechanisms associated with AD, making it a relevant therapeutic target, particularly due to its involvement in signaling pathways related to tau pathology and neuronal dysfunction. In this context, proteolysis-targeting chimeras (PROTACs) have emerged in the literature as a promising strategy for the selective degradation of GSK-3β, particularly due to their ability to promote sustained target depletion rather than transient inhibition. Several candidate PROTACs capable of recruiting GSK-3β to the E3 ubiquitin ligase cereblon (CRBN) have been synthesized and evaluated by Jiang et al. (2021), highlighting the importance of efficient ternary complex formation for productive ubiquitination and subsequent proteasomal degradation. In this sense, the stability and geometry of the ternary complex are considered key determinants of PROTAC efficacy and selectivity. In this work, we propose a conformational search approach combined with protein–protein docking to predict GSK-3β–PROTAC–CRBN ternary complexes. This computational strategy allows the exploration of multiple binding modes and relative orientations between the target protein, the PROTAC molecule and the E3 ligase, providing structural insights into cooperative interactions that may favor ternary complex stabilization. Correlation of our computational results with experimental data is expected to refine the rational design of PROTACs, contributing to a deeper molecular understanding of the structural and interaction features that govern PROTAC efficiency, and supporting the development of more effective degraders with potential application in the treatment of AD.

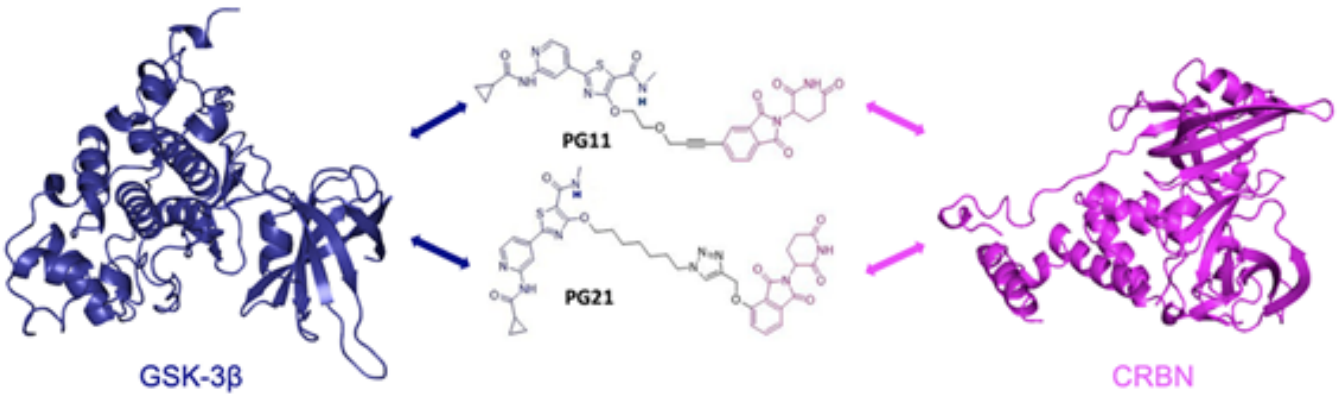


Figure 1. GSK-3b, CRBN and two of the best ranked PROTACs developed by Jiang et al. (2021).

Agradecimentos/Acknowledgments

The authors are grateful to the Military Institute of Engineering (IME) for infrastructure and CAPES, CNPq and INCT-Defesa for financial support.

Theoretical Insights into the Inactivity of Arylboronic Derivatives Against the Proteasome

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Palavras Chave:*Proteasome,Boronic acids,QM/MM methods,Molecular reactivity,Drug design*

Highlights

Comparative study reveals why alkylboronic compounds outperform arylboronic analogues

Resumo/Abstract

The proteasome is a validated therapeutic target whose inhibition occurs through the formation of a tetrahedral intermediate resulting from the nucleophilic attack of the catalytic threonine residue (Thr1) on the boronic acid moiety. Previously evaluated arylboronic derivatives did not exhibit significant inhibitory activity against the proteasome (**Table 1**), suggesting that structural and electronic factors influence the reactivity of the boron atom.

In order to investigate the molecular basis of this behavior, a comparative analysis was performed between the arylboronic fragment of**LASSBio-2391**and its analogue containing a reduced ring**1**, using semiempirical calculations with the MOPAC program at the PM7 level (**Figure 1**).

The results indicated that the reduction of the aromatic ring promotes structural changes that favor the nucleophilic approach of threonine to the boron atom (**Figure 1**). The system containing the reduced ring showed a greater predisposition to form the tetrahedral intermediate when compared to the aromatic system, suggesting that the π-conjugation of the aromatic ring contributes to the stabilization of the boron center and consequently reduces its reactivity.

These results provide a molecular explanation for the lack of activity observed in arylboronic derivatives and indicate that structural modulation of the ring adjacent to the boronic acid moiety may be a determining factor for reactivity toward the catalytic site of the proteasome. Additional studies employing hybrid QM/MM approaches are currently underway to provide a more detailed energetic description of the ligand–enzyme interaction process

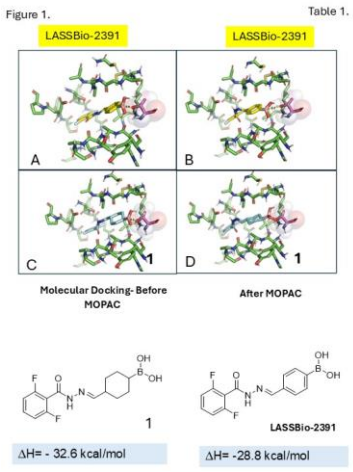


Table 1.

Compound	% Maximum inhibition (10 μM)
LASSBio-2391	16.79
LASSBio-2394	8.77
LASSBio-2395	0
LASSBio-2393	4.94
LASSBio-2396	16.64
LASSBio-2397	1.72
LASSBio-2392	0
Ixazomibe	90

Figure 1MOPAC semi-empirical calculations using PM7 hamiltonian. Table 1 Inhibitory activity again

Agradecimentos/Acknowledgments

The authors would like to thank the Central Analytical – LAMAR of the Institute of Natural Products for the analytical support. We also acknowledge INCT-INOFAR and CNPq for the financial support.

The Role of Protein Kinase MARK4 in Neurodegenerative Diseases: A Virtual screening Study from PeQuiM'S Library

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Palavras Chave:*Drug discovery,virtual screening,MARK4,neurodegenerative disease*

Highlights

MARK4 drives Tau hyperphosphorylation in AD.

PeQuiM library screened against MARK4.

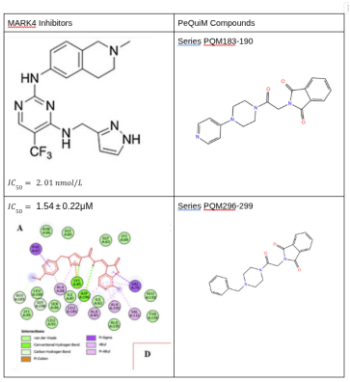
DockThor docking identified promising inhibitors.

Hits show neuroprotective potential and feasible synthesis.

Resumo/Abstract

Microtubule affinity-regulating kinases (MARKs) comprise four isoforms (MARK1–4), which are highly enriched in the human brain. MARK4 (microtubule-associated protein/microtubule affinity-regulating kinase 4) is a serine/threonine kinase involved in the phosphorylation of microtubule-associated proteins (MAPs) that regulate microtubule dynamics. Aberrant MARK4 activity has been proposed to contribute to neurofibrillary tangle formation in Alzheimer's disease (AD). Structurally, MARK kinases consist of three main regions: a kinase domain, a ubiquitin-associated (UBA) domain, and a short linker sequence. The overexpression of MARK4 in AD brains promotes the phosphorylation of Tau protein at KXGS motifs, leading to Tau hyperphosphorylation and subsequent formation of neurofibrillary tangles. Moreover, MARK4 overexpression has been associated with a pro-inflammatory state, particularly under pathological conditions of the central nervous system. In this context, the present study aimed to perform a comparative analysis among several compounds developed at the Medicinal Chemistry Research Laboratory (PeQuiM) for neuroprotective purposes with known MARK4 inhibitors. Computational screening and molecular docking (using the Dockthor platform) were employed as methodological approaches, aiming to identify promising candidates that may support the development of potent MARK4 inhibitors through feasible synthetic routes.

Guedes, I. A.; Pereira da Silva, M. M.; Galheigo, M.; Krempser, E.; de Magalhães, C. S.; Correa Barbosa, H. J.; Dardenne, L. E.*DockThor-VS: A Free Platform for Receptor-Ligand Virtual Screening*. Journal of Molecular Biology 2024, 168548.**LI, Fangfang**et al. PCC0208017, a novel small-molecule inhibitor of MARK3/MARK4, suppresses glioma progression*in vitro*and*in vivo*.**Acta Pharmaceutica Sinica B**, Beijing, 2020.



Structural mapping of potent MARK4 inhibitors (IC_{50}) and comparison with the PeQuiM series.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge financial support from the Brazilian research funding agencies FAPEMIG, CAPES, CNPq, FINEP and INCT, and computational resources provided by the National Laboratory for Scientific Computing (LNCC).

Triagem Virtual da Quimioteca do PPGQ-UFRRJ para a Busca de Candidatos a Inibidores de Leishmanolisina de Leishmania spp

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Palavras Chave:*Leishmaniose; GP63; Docagem molecular; Triagem Virtual; Metaloprotease*

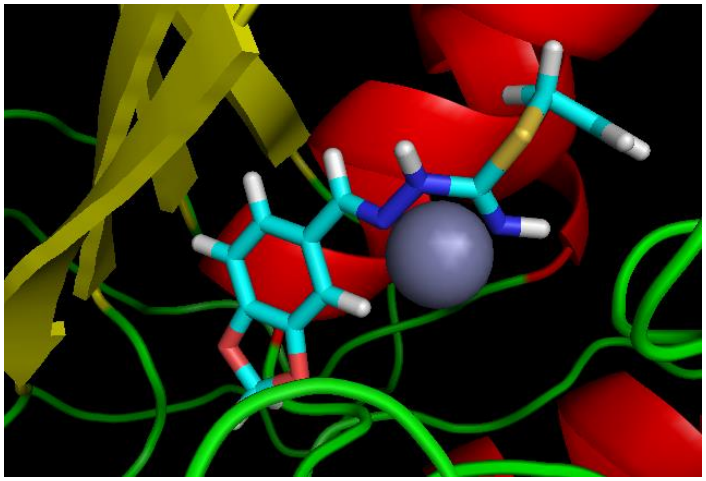
Highlights

Virtual screening by molecular docking identified promising*Leishmania*GP63 inhibitors in the PPGQ-UFRRJ chemical library with interesting lead-like properties.

Resumo/Abstract

As leishmanioses constituem um complexo de doenças infectoparasitárias causadas por protozoários do gênero Leishmania. A enfermidade ocorre em três formas clínicas principais: cutânea, mucocutânea e visceral, a qual, se não tratada, é fatal em mais de 95% dos casos. Estima-se que 50.000 a 90.000 novos casos de LV ocorram anualmente em todo o mundo. Diante da inexistência de vacinas eficazes e de limitações da quimioterapia atual, a busca por novas opções terapêuticas torna-se urgente. Nesse contexto, a glicoproteína GP63, ou leishmanolisina, uma metaloprotease de zinco encontrada majoritariamente na superfície do parasita, é um candidato a alvo molecular promissor devido ao seu papel crucial na virulência, invasão celular e evasão do sistema imune.

Este trabalho teve como objetivo identificar novos candidatos a inibidores da GP63 na quimioteca do PPGQ-UFRRJ, com mais de 700 compostos cadastrados, utilizando estratégias de Triagem Virtual Baseada na Estrutura (SBVS). A metodologia empregou a docagem molecular com o programa GOLD (função GoldScore), em duplicata, na estrutura cristalográfica da leishmanolisina (código 1LML no PDB, resolução de 1,86 Å). Os compostos com as 50 melhores pontuações foram submetidos à predição das propriedades farmacocinéticas e toxicológicas utilizando-se o servidor SwissADME para se refinar os resultados com enfoque nos limites físico-químicos que definem um bom composto líder, ou seja, uma entidade molecular adequada para otimização, útil para o planejamento de novas séries de candidatos a inibidores. Desta análise, destacaram-se 5 padrões estruturais. Um desses padrões contém o grupo hidrazinacarbimidotioato, que se mostrou bastante promissor devido à sua capacidade de atuar como ligante bidentado sobre o íon Zn(II) catalítico (fig. 1). Cálculos quânticos com o método semi-empírico PM7 para otimização total da geometria de interação do sistema enzima-ligante confirmaram esse padrão de interação e a estabilidade do complexo.



Modo de interação bidentado de derivado hidrazinacarbimidotioato (bastões) como íon Zn(II) (esfera)

Agradecimentos/Acknowledgments

CAPES, FAPERJ, CNPq

UNCOVERING THE HIDDEN BIOACTIVITIES OF COMPOUNDS: EU-OPENSCREEN's OPEN COMPOUND SHARING INITIATIVE

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Palavras Chave:*compound collection, compound sharing, collaborations, bioactivities, drug discovery*

Highlights

EU-OPENSCREEN's open compound sharing initiatives allows chemists to expose their compounds to a variety of biological/drug targets to collaboratively uncover the bioactivities of their compounds.

Resumo/Abstract

Chemists produce many compounds to modulate specific activities of certain target or phenotypes. But only a few individual compounds, e.g., those most active in a specific assay, are used in further studies, while most of these compounds are stored on shelves and in fridges unused, despite the considerable effort in time and resources that was invested in making them. Furthermore, compounds with low activity against the target, for which they have been synthesized, may be active and useful against another target or in an unrelated assay. Unfortunately, for chemists, who synthesized these compounds, the opportunities are limited to systematically test their compounds against a wide variety of biological targets in order to uncover these hidden biological activities.

With the aim of allowing chemists to uncover novel bioactivities of their compounds, the publicly funded initiative EU-OPENSCREEN enables chemists to make their compounds available, in a regulated and transparent framework, to other biologists, who test these compounds in suitable bioassays. Chemists thereby expose their compounds to various biological/drug targets to uncover compounds' unknown bioactivities, which would otherwise not be practical through individual one-to-one collaborations. Once a compound shows activity in a specific assay, a research collaboration between the chemist and the assay provider can be initiated.

EU-OPENSCREEN (www.eu-openscreen.eu) supports discovery projects in early drug discovery by democratizing access to technology platforms, expertise and compound collections and by creating a pre-competitive network of like-minded researchers. EU-OPENSCREEN's ca. 30 academic partner institutions offer complementary expertise and capabilities to collaboratively develop novel chemical probes for the life sciences community. Primary screening data are made available to the scientific community through its open-access European Chemical Biology Database (https://ecbd.eu/).

Agradecimentos/Acknowledgments

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Unveiling the Pharmacological Potential of Ts3 from scorpion venom: Computational Insights into Muscarinic M2 Receptor Activation

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Palavras Chave:*Scorpion Envenomation,Molecular Modeling,Tityus serrulatus,Muscarinic M2 Receptor,Ts3*

Highlights

This research aims to study and develop the modeling interaction between Ts3 toxin and muscarinic M2 receptor, intending to explore an alternative treatment for effects of*Tityus serrulatus*venom.

Resumo/Abstract

Scorpionism is classified as a neglected tropical disease by the World Health Organization (WHO), disproportionately affecting marginalized areas. In Brazil,*Tityus serrulatus*is responsible for the majority of scorpion-related accidents, with acute pulmonary edema being the primary cause of death in severe cases. Consequently, the development of novel therapeutic strategies capable of mitigating envenomation effects before serum administration is of great pharmacological interest[1]. Therefore, this study explores the potential of the Ts3 toxin, a component of*Tityus serrulatus*venom, as an agonist of the muscarinic M2 receptor (M2R)[2]. The docking methodology was validated using re-docking on a restricted binding site, yielding RMSD of 0.1605 Å and an energy score of -178.56. Interactions between M2R and the toxin's terminals were assessed via the HDOCK server, identifying optimal complexes with energy scores of -92.79 (C-terminal) and -71.30 (N-terminal)[3]. Subsequently, Molecular Dynamics (MD) simulations were performed using those C- and N- terminals in aqueous solution using GROMACS 2025.3 with the AMBER03 force field[4]. The system was solvated in a triclinic box with a 1.2 nm buffer at neutral pH. The production run was analyzed for 100 ns to ensure structural convergence. Thermodynamic parameters were monitored, maintaining an average temperature of 309.956 K (N-terminal) and 309.976 K (C-terminal). Structural stability was evaluated through RMSD, Radius of Gyration, and Root Mean Square Fluctuation (RMSF) graphs. The next steps in the research will be the dynamics of the complex with M2R and the membrane.

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49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

ORG - Química Orgânica

1,2,3-TRIAZOLIL-4-HIDROXÂMICOS COMO PLATAFORMAS SINTÉTICAS PARA A CONSTRUÇÃO DE NOVOS COMPLEXOS METALOCOROAS

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Palavras Chave:*Metallacrowns,Triazóis,Compostos de coordenação,Click Chemistry,Metais de transição*

Highlights

New triazole-based hydroxamato ligands for metallacrown synthesis.

Click chemistry as a versatile route to new molecular materials.

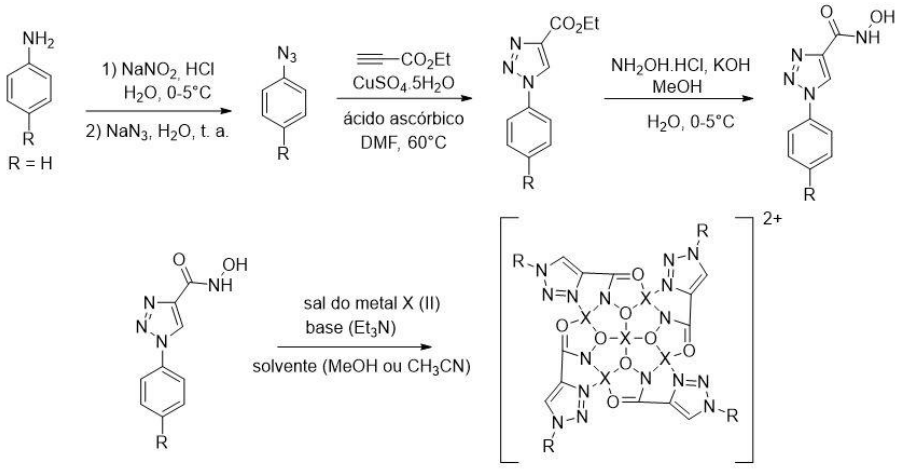
New Cu(II) and Ni(II) metallacrowns.

Resumo/Abstract

Desde os estudos pioneiros de Charles Pedersen, em 1967, os éteres de coroa têm desempenhado papel central no desenvolvimento da química supramolecular, destacando-se por sua capacidade de coordenação seletiva de íons metálicos. Como análogos inorgânicos desses sistemas, as metalocoroas (*metallacrowns*, MCs) são compostos metalomacrocíclicos formados por unidades repetidas envolvendo átomos metálicos, nitrogênio e oxigênio, apresentando elevada estabilidade estrutural e aplicações potenciais em magnetismo molecular, luminescência, catálise e reconhecimento molecular.

A síntese desses sistemas baseia-se majoritariamente em ligantes derivados de ácidos hidroxâmicos, cuja desprotonação favorece a coordenação metálica. Nesse contexto, este trabalho propõe a síntese de novos pró-ligantes ácidos 1,2,3-triazolil-4-hidroxâmicos visando sua conversão em sistemas metalocoroas. Os substratos 1,2,3-triazólicos foram obtidos por reação de cicloadição azida–alcino catalisada por Cu(I) (CuAAC), conhecida por sua robustez, regioespecificidade e altos rendimentos. A reação entre azidas aromáticas e propiolato de etila forneceu ésteres triazólicos intermediários, posteriormente convertidos nos respectivos ácidos hidroxâmicos por reação com hidroxilamina.

Os pró-ligantes foram caracterizados por espectroscopia no IV e RMN de ^{1}H e ^{13}C. Tentativas de obtenção de derivados metalocoroas centrados em Cu(II) e Ni(II) foram realizadas pela reação dos pró-ligantes com sais metálicos na presença de Et_3N. Embora os espectros no IV sugiram a formação de complexos metálicos, ainda não foi possível obter monocristais adequados para caracterização estrutural inequívoca por difração de raios X. Estudos adicionais de cristalização encontram-se em andamento.



Agradecimentos/Acknowledgments

Agradecimento às agências de fomento CAPES, CNPQ e FAPERJ

A Bunte Salt-Based Strategy for Accessing New Thiolactone Scaffolds from Dihydropyrimidinones

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Palavras Chave:*Dihydropyrimidinone,Bunte salts,Green chemistry,Thiolactones*

Highlights

Multicomponent synthesis of DHPMs enabled the synthesis of novel thiolactones from Bunte salts (S-alkyl thiosulfates), offering an efficient and organometallic-free approach with high atom economy.

Resumo/Abstract

Multicomponent reactions (MCRs) represent an important strategy for the development of new compounds, as they promote high atom economy and reduced waste generation during synthetic processes. In this context, the dihydropyrimidinone (DHPM) scaffold stands out as a versatile platform accessible via MCRs, allowing diverse structural modifications and exhibiting a wide range of reported biological activities.[1] In this work, Bunte salts are employed as viable sulfur precursors for the synthesis of novel thiolactones derived from DHPMs, avoiding conventional organometallic approaches.[2] Based on previous studies developed by our research group, reaction parameters, including reducing agent, stoichiometry, temperature, solvent, and workup, were systematically optimized. All compounds were fully characterized by 1D and 2D NMR spectroscopy, and novel derivatives were further confirmed by HRMS. The DHPM–Bunte intermediates (2a–2e) were obtained in high isolated yields (85–92%), while the corresponding thiolactones (3a–3e) were formed in moderate to excellent yields (26–89%) (Fig. 1). Overall, this methodology provides an efficient, organometallic-free route to thiolactone scaffolds from DHPMs, aligning with principles of green chemistry.

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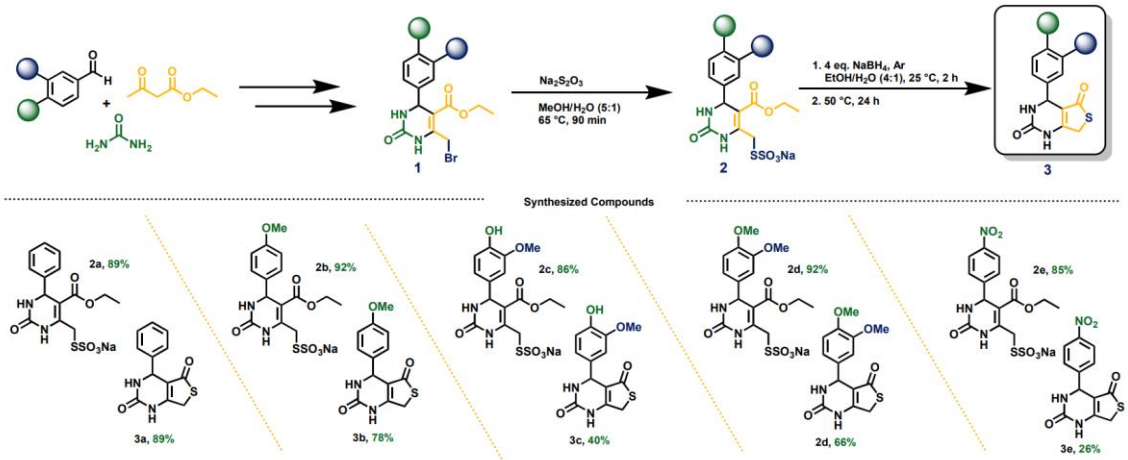


Fig. 1. General route to thiolactones from Bunte salts and yields.

Agradecimentos/Acknowledgments

We gratefully acknowledge financial support from CAPES, CNPq, and FAPESC.

Advances on the enantioselective synthesis of Leucoptera sinuella (Reutti, 1853) sex pheromone employing Evans Oxazolidinones as chiral auxiliaries.

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Palavras Chave:*semiochemicals,enantioselective synthesis,asymmetric synthesis,chiral auxiliary,Leucoptera sinuella*

Highlights

Evans auxiliary strategy targets stereocontrolled access to all 3,7-dimethylpentadecane isomers.

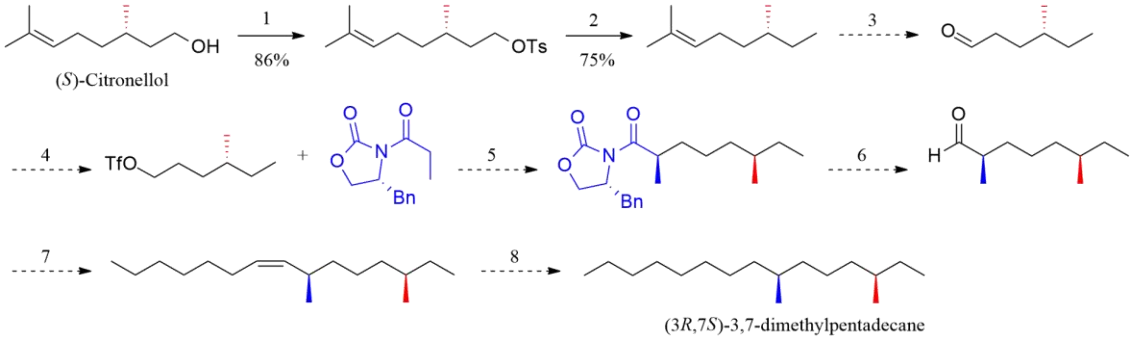
Wittig-based endgame delivers stereopure pheromone candidates for absolute-configuration assignments.

Resumo/Abstract

Leucoptera sinuella (Lepidoptera: Lyonetiidae; “Scotch bent-wing moth”) has emerged as an invasive leaf-miner in Chile, impacting yields of fruit-producing trees[1]. The female-produced sex pheromone 3,7-dimethylpentadecane was reported in 2020[2]; its methyl-branched framework prevented chiral resolution, and the pheromone was evaluated as a stereoisomeric mixture. To enable absolute-configuration assignment and support pheromone-based management, we are developing a stereocontrolled synthesis of the individual stereoisomers of 3,7-dimethylpentadecane.

Progress to date has focused on the (S)-β-citronellol branch. Tosylation proceeded in 86% yield, and reduction afforded 2,6-dimethyl-2-octene in 75% yield, providing a convergent intermediate for downstream stereodivergence. To access the required aldehyde fragment, photocatalyzed oxidative C=C cleavage using 4-nitrobenzonitrile is being evaluated as an operationally simple alternative to ozonolysis, targeting 4-methylhexanal, then reduced to the corresponding alcohol. For stereocontrolled methyl installation, coupling of the prepared triflates with the (R)-Evans auxiliary is designed to set the configuration at the internal methyl-bearing center; auxiliary removal/hydrolysis furnishes the diastereomeric aldehydes (2R,6S)- and (2R,6R)-2,6-dimethyloctanal. These aldehydes are advanced via Wittig olefination with heptanal, followed by reduction, to deliver the pheromone stereoisomers (3S,7S)- and (3R,7S)-3,7-dimethylpentadecane. The complementary (3S,7R) and (3R,7R) diastereomers are accessed by switching to the enantiomeric Evans auxiliary. Overall, this modular approach aims to provide a complete stereoisomer set for unambiguous configuration assignment and comparative behavioral evaluation.

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Leucoptera sinuella (Reutti, 1853)

Agradecimentos/Acknowledgments

The authors would like to thank CAPES, CNPq and INCT - BioInnovations for sustainable agriculture for funding.

Advances on the enantioselective synthesis of Prionus californicus sexual pheromone employing Evans Oxazolidinones as chiral auxiliaries

Eduardo Cordeiro (PG)*[1], Eron Rafael Ferreira Bueno dos Santos (IC)[1], Alana Vitoria Machado (IC)[1], Giuliana Pavaneli (PQ)[1], Paulo Henrique Gorgatti Zarbin (PQ)[1].

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Palavras Chave:*natural products; semiochemicals; Prionus californicus; enantioselective synthesis; oxazolidinones.*

Highlights

In this work, we used Evan's oxazolidinone to control stereochemistry in pheromone synthesis. This study should contribute to applications in integrated pest management in agriculture.

Resumo/Abstract

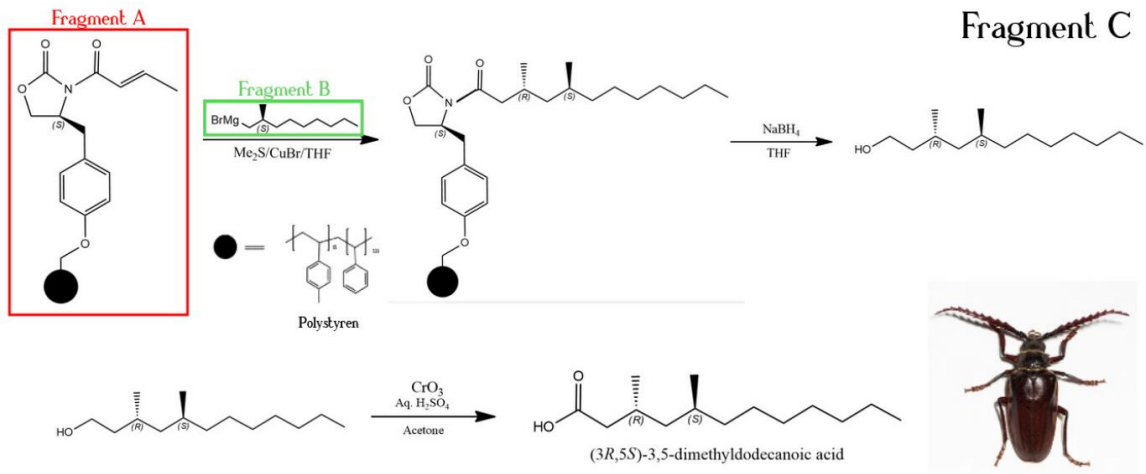
Prionus californicus, is a difficult-to-control pest in fruit tree crops. Recent studies led to the first identification of the female-produced sex pheromone of this insect. The structure was determined to be an isomer of 3,5-dimethyldodecanoic acid. The synthesis of this molecule as a mixture of all four possible stereoisomers, followed by field tests, successfully confirmed the discovery.[1]

To confirm the hypothesis that the mixture of the four stereoisomers is responsible for attracting the beetle, the following work aims to carry out the enantioselective synthesis of the isomers of (3R,5S)-3,5-dimethyldodecanoic acid. To achieve this objective, a convergent synthesis strategy was adopted, dividing the target molecule into three main building blocks, which we call fragments A, B, and C, using Evans' oxazolidinones as chiral inducers.[2]

In Fragment A, we are producing an Evans oxazolidinone derived from L-tyrosin to a polymer-supported Evans auxiliary[3]. In Fragment B, we are also producing an Evans oxazolidinone[2] starting from L-phenylalanine followed by acylation, beta-alkylation, and finally, a reduction and an Appel reaction to form the desired alkyl bromide. In Fragment C, the key step is a Grignard reaction between the (S)-1-bromo-2-methylnonane, and the styrene-supported oxazolidinone from Fragment A followed by another reduction step and, finally, a Jones oxidation to form the carboxylic acid, yielding the final pheromone.[4]

Now we synthesized oxazolidinone from L-phenylalanine (a, 91%) and L-tyrosin (b, 83 %) followed by acylation (c, 80%), beta-alkylation (d, 70%) and the reduction (e, 95%) of the fragment B.The next steps are to synthesize the polystyrene-supported chiral auxiliary and complete the synthesis of the pheromone.

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Fragment C of the synthesis with a photo of Prionus californicus

Agradecimentos/Acknowledgments

The authors would like to thank CAPES, CNPq and INCT for funding

Aggregation-Induced Emission and Solvatochromic Behavior of 2,3-Arylquinoxaline-6-Carboxylic Acid Derivatives

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Palavras Chave:*Quinoxalines,Solvatochromism,Luminescence,Organic Materials,Aggregation-Induced Emission*

Highlights

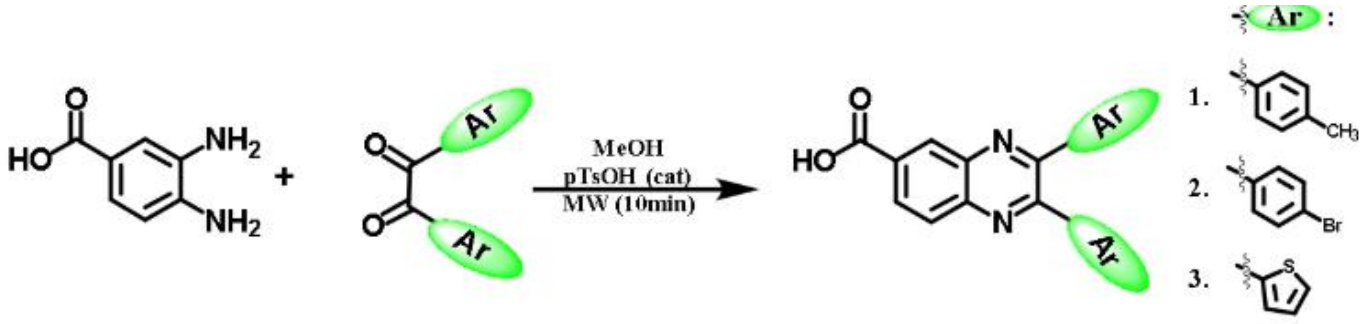
The photophysical behavior of quinoxaline derivatives is governed by the aryl substituents. Molecules have strong solvatochromism and AIE in THF/H_2O systems, with fluorescence enhanced by aggregation.

Resumo/Abstract

Quinoxaline derivatives have attracted considerable interest as organic luminophores due to their tunable electronic structures and solid-state emissive properties, contributing to the development of innovative functional materials for optoelectronic and optical sensing applications. In this study, three 2,3-arylquinoxaline-6-carboxylic acid derivatives were synthesized via condensation reactions between 3,4-diaminobenzoic acid and aromatic 1,2-dicarbonyl substituents (**Scheme 1**). Structural characterization was achieved by IR and ^{1}H/ ^{13}C NMR spectroscopy.

The photophysical properties were investigated by UV–Vis absorption and fluorescence spectroscopy in solution and in the aggregated state. All compounds exhibited intense absorption bands and fluorescence emission, strongly dependent on the nature of the aryl substituent. The thienyl-substituted derivative (**3**) displayed the most pronounced bathochromic shifts and higher fluorescence efficiency (**ϕ**= 4.6%; $\lambda_{abs,max}$ =392 nm; $\lambda_{em,max}$ = 463 nm), consistent with an enhanced push–pull electronic system and in agreement with trends reported for quinoxaline-based luminophores in the literature. Solvatochromic studies revealed positive solvatochromism, indicating stabilization of a polar excited state in polar media.

Aggregation-induced emission (AIE) was observed in THF/water mixtures, with a marked increase in emission intensity upon aggregation, particularly for the*p*-tolyl derivative (**1**), which showed up fluorescence enhancement. This behavior, was attributed to the restriction of intramolecular rotation of phenyl rings at the 2,3-positions of the quinoxaline core, effectively reducing non-radiative decay pathways. These results demonstrate that subtle variations in aryl substituents efficiently modulate the luminescent properties of quinoxaline derivatives, reinforcing their potential for optoelectronic and sensing applications within the context of sustainable technological innovation.



Scheme 1: Synthesys of target molecules 1-3.

Agradecimentos/Acknowledgments

CNPq, CAPES and FAPESQ-PB

A Low-impact Mechanochemical Method for the Synthesis of 5-Amino-1H-1,2,3-triazoles under Solvent-free Conditions

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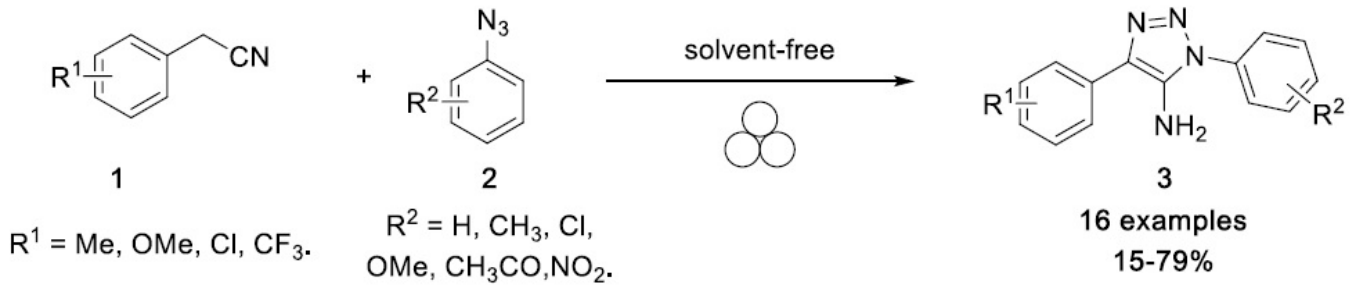
Palavras Chave:*: 5-amino-1,2,3-triazoles; solvent-free; Mechanochemistry,5-amino-1,2,3-triazoles,solvent-free,Mechanochemistry*

Highlights

Broad-Scope Mechanosynthesis of 5-Amino-1*H*-1,2,3-triazoles Scaffolds Significance in Medicinal Chemistry Solvent-free Conditions

Resumo/Abstract

5-amino-1,2,3-triazoles exhibit significant biological activities, including anticancer, antifungal, antitrypanosomal and antiherpesvirus properties [1]. Several methods for the synthesis of these triazoles have been reported, often employing toxic solvents or hash reaction conditions [2]; alternatively, eco-friendly approaches such as ionic liquids and solvent-free protocols have been described [3,4]. However, these methods suffer from notable drawbacks, including limited substrate scope, long reaction times, restricted reactant compatibility, and laborious workup procedures. Herein, we report a new green methodology for the synthesis of a series of 5-amino-1,2,3-triazoles**3**from arylacetonitriles**1**and arylazides**2**in the presence base and milling auxiliary under mechanochemical conditions (Scheme 1). This approach affords the desired products with a broad substrate scope (16 examples, 15-79% yields), without limitation related to the physical state of the reactants (liquids or solids). The method is tolerant of a wide range of substituents, including both electron-withdrawing and electron-donating groups, as well as the acetyl functional group. The protocol including low mechanical energy impact, simple, rapid, and cost-effective, enabling facile product isolation by column filtration. Notably, it provides access to 14 unexplored compounds. To the best of our knowledge, this methodology represents the first mechanochemical approach for the synthesis of 5-amino-1,2,3-triazole derivatives at room temperature under rapid reaction conditions.



Synthesis of 5-amino-1H-1,2,3-triazoles via mechanochemistry under solvent-free conditions.

Agradecimentos/Acknowledgments

CNPq, FAPERJ, UnB

Amino-Naphthoquinones Synthesis using Silica Supported Copper Catalyst

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Palavras Chave:*Amino-Naphthoquinone,Oxidative coupling,Supported copper catalyst.,Supported copper catalyst*

Highlights

Amino-naphthoquinones synthesis by oxidative coupling using supported copper catalyst was presented as a green synthetic route. The synthesis showed 96% yield and recyclability of the catalyst.

Resumo/Abstract

Naphthoquinones belong to the family of quinones, a family of molecules with known pharmacological properties [1]. Lapachol is the best-known naphthoquinone and has numerous biological activities, including anti-cancer activity [2]. In parallel, the synthesis of amino-naphthoquinones derivatives using copper acetate as a catalyst in an acidic environment presents itself as an efficient and robust approach to obtain this class of compounds. Heterogeneous catalysis using metal/silica hybrid materials appears to be an important strategy for reducing impacts on the environment, mainly due to recyclability [3].
In a Green Chemistry approach, we propose 2-(Phenyl)amino-1,4-naphthoquinone synthesis using Cu/SO_2 catalyst as a response to Copper(ll) Acetate [1], and the Cu/SO_2 synthesis via Sol-Gel process. The reaction was carried out in a continuous flow in new glassware, optimized by varying solvent, heat, Cu/SO_2 mass and time, which led yields up to 96%. The product was followed by IR Spectroscopy, NMR, melting point. The morphology of Cu/SO_2 was investigated by scanning electron microscope(SEM) and Energy-dispersive X-ray spectroscopy (EDX). The reaction optimization and catalyst recycle has successfully been done, currently the following steps will be vary the amines to test the reaction robustness.

Table 1 - Optimization of the reaction to synthesize 2(Phenyl)amino-1,4-naphtoquinone

Entry	Catalyst (mol%)	Temperature (°C)	Solvent	Time (min)	Yield (%)
1	5	60	AcOH	40	76
2	10	60	AcOH	40	96
3	20	60	AcOH	40	90
4	10	80	AcOH	40	96
5	10	Room Temperature	AcOH	40	Not occur
6	10	60	EtOH	40	75
7	10	60	ACN:(4):(1) AcOH	40	Not occur
8	10	60	H_20	40	Multiple by products
9	10	60	DMSO	40	Multiple by products
10	10	60	AcOH	10	33
11	0	60	AcOH	120	49

Table 1 - Optimization of the reaction to synthesize 2(Phenyl)amino-1,4- naphtoquinone

Agradecimentos/Acknowledgments

We would like to thank the Instituto Multidisciplinar de Química, Centro Multidisciplinar UFRJ-Macaé.

A new mechanochemical approach using a vortex for the synthesis of 6,8-dichloroquercetin and its preliminary characterization via FT-IR

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Palavras Chave:*Flavonoids Quercetin,Chlorination,Mechanochemistry,Flavonoids,Quercetin*

Highlights

Low-cost mechanochemical chlorination of quercetin using a vortex mixer. Green synthesis of chlorinated flavonoids without solvents or expensive equipment. Formation of C-Cl bonds on quercetin.

Resumo/Abstract

Flavonoids are polyphenolic compounds produced from phenylpropanoids and are widely distributed in plant species and some microorganisms. They usually present a structure containing 15 carbon atoms.[1] Quercetin is a flavonol with hepatoprotective and nephroprotective properties, as well as high antioxidant activity. The introduction of chlorine atoms into the A ring of this flavonoid can enhance its antioxidant capacity.[2] In this context, mechanochemistry using a vortex mixer can be a low-cost alternative for the synthesis of flavonoid derivatives, complying with some principles of green chemistry, in addition to enabling reactions that are not possible using traditional methods, which often require high-cost equipment.[3] In this method, a Falcon tube containing three stainless steel spheres was used, quercetin (0,165 mmol, yellow solid, melting point 316-317 °C) and trichloroisocyanuric acid (0,165 mmol) were added to the same tube, which was then agitated using a vortex mixer for 2 hours with agitation speed at level 4. Obtaining an orange solid (70% conversion rate, melting point 276-277 °C). IR spectrum analysis showed a band at ~690 cm-1 corresponding to the C-Cl stretching, in addition to the absence of out-of-plane C-H angular deformation bands, due to the hexassubstituted pattern of ring A. The preliminary data obtained are promising and demonstrate the potential of the method, enabling the use of mechanochemical techniques through a fast and low-cost methodology, verified according to the principles of green chemistry.

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Applying mechanochemistry to SNAr of 1,2-dichloro-4-nitrobenze with alcohols.

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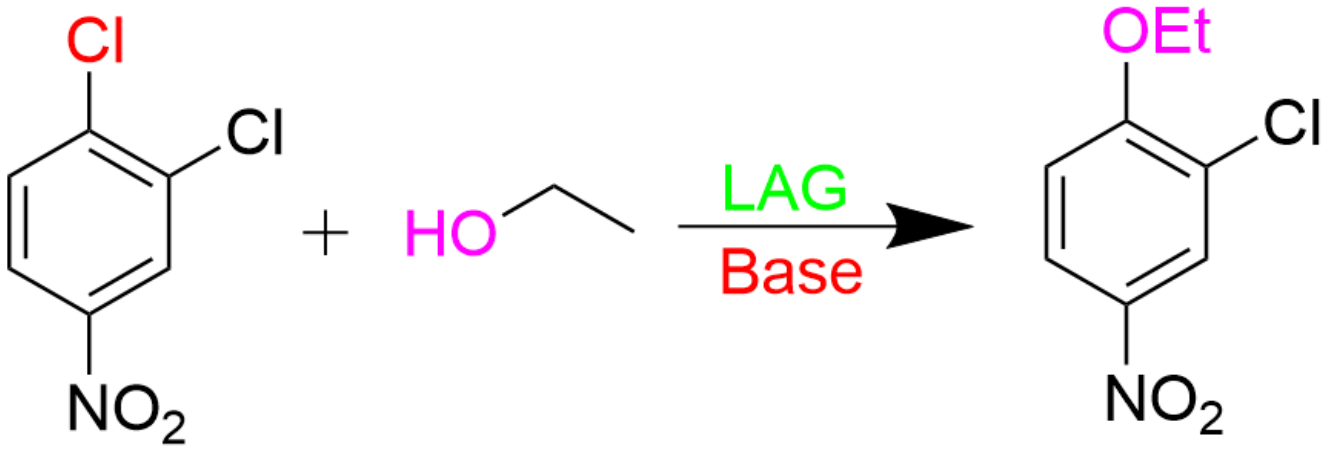
Palavras Chave:*mechanochemistry, nucleophilic aromatic substitution, green chemistry.*

Highlights

Mechanochemistry enables greener SNAr with ethanol, achieving up to 80% conversion to the product.

Resumo/Abstract

Mechanochemistry is a green chemical method that offers a sustainable alternative to condensed-phase synthesis, minimizing the use of solvents, reducing reaction time, and enabling the use of poorly soluble reagents. The method has been used in several areas, particularly in organic synthesis. Furthermore, aromatic nucleophilic substitution stands out for introducing functional groups into aromatic rings, generating key intermediates for pharmaceuticals. Recently, a mechanochemical method for the nucleophilic aromatic substitution of aryl fluorides by nitrogen nucleophiles with no base and as an auxiliary milling has been developed. However, the use of alcohols and thiols as nucleophiles is still unexplored so far via mechanochemistry. Therefore, this work aims to evaluate alcohols as nucleophiles in the mechanochemical SNAr, expanding the scope of this method. The experiments were carried out in a vibrational mill, Retsch MM 200, varying parameters as stoichiometry, milling time, bases, order addition, and liquid assisted grinding (LAG). The reaction of 1,2-dichloro-4-nitrobenzene and ethanol has been evaluated with different bases and solvents as LAGs. Preliminary results indicate that use of NaOtBu as base, DMF as LAG, using a prior agitation before adding the base was essential for the formation of the product, reaching up to 80% of conversion to the desired product and 20% of starting material. In addition, the increase in grinding time resulted in total consumption of the substrate; however, a decrease in the yield of the product of interest, and the appearance of by-products (still unidentified) was observed. Another relevant advantage is the easy isolation of the product by recrystallization in isopropyl alcohol, with spectroscopic data consistent with the literature. Additional studies are underway to identify the observed by-product and to apply chemometric tools in the optimization of the experimental conditions, aiming at maximizing the reaction yield.



Main reaction with ethanol as nucleophile

Agradecimentos/Acknowledgments

CAPES, FACEPE CNPq, UFPE e CA-dQF

A SIMPLE AND PRACTICAL ACCESS TO UNPRECEDENTED C-3 N-FUNCTIONALIZED INDOLIZINES

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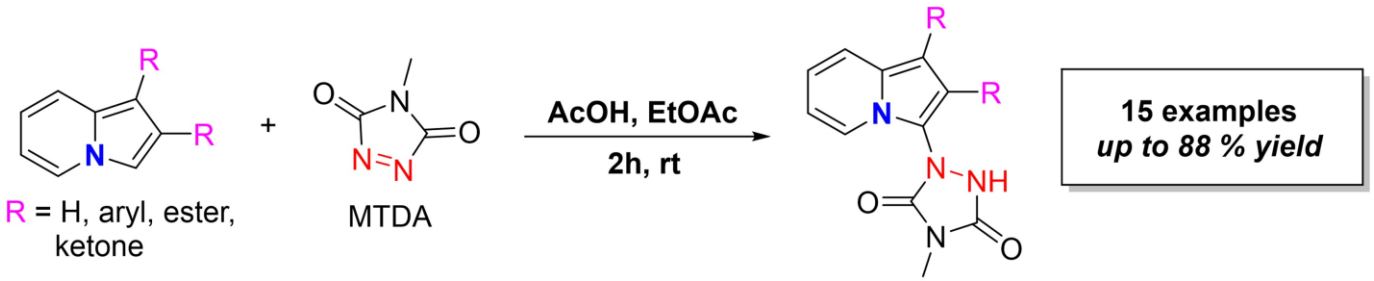
Palavras Chave:*Indolizine,Amination,Urazole,Heterocycle*

Highlights

A selective strategy for indolizine N-functionalization enables access to unprecedented heterocyclic scaffolds under simple, mild and sustainable conditions.

Resumo/Abstract

Indolizines are privileged heteroaromatic scaffolds with growing importance in medicinal chemistry and materials science[1]. Among the various transformations applied to aromatic systems, electrophilic amination reactions represent a powerful tool for introducing nitrogen functionalities, which can significantly impact the biological and physicochemical properties of the resulting molecules.[2] However, methodologies for direct C–N bond formation on indolizines remain scarce. In this work, we explored the electrophilic N-functionalization of indolizines using MTAD as an efficient and highly reactive agent. The strategy enabled the successful functionalization of the indolizine core under mild conditions, providing unprecedented 3-substituted derivatives in moderate to good yields (Secheme 1). A systematic evaluation of substituent effects demonstrated that electron-donating groups enhance reactivity at the C-3 position, while electron-withdrawing groups, particularly nitro substituents, drastically reduce product formation. Remarkably, the methodology showed high selectivity for the indolizine ring over other aromatic sites, even in electronically activated substrates. Despite challenges regarding product instability during purification, the protocol allowed the isolation of a diverse library of aminated indolizines, highlighting MTAD as a powerful electrophilic aminating agent for this important class of heterocycles under simple, mild and environmentally friendly conditions.



Scheme 1

Agradecimentos/Acknowledgments

This study was financed by theCoordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001 and São Paulo Research Foundation (FAPESP), grants 2022/16916-3, 2024/01253-4, and 2022/05327-7.

A Synzyme-Based Approach for the Synthesis of Tetrazolo[1,5-a]pyrimidine Derivatives Using Polyethyleneimine and Ionic Liquids

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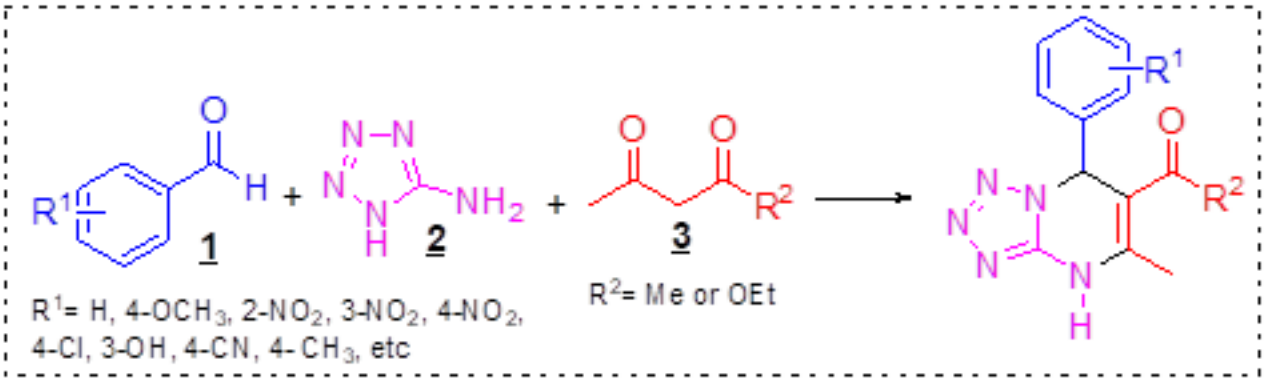
Palavras Chave:*Multicomponent reactions, tetrazoles, biological activities*

Highlights

Tetrazolo[1,5-a]pyrimidine derivatives were efficiently synthesized using an ionic liquid catalyst, providing a simple and versatile route to biologically relevant scaffolds.

Resumo/Abstract

Tetrazoles fused to pyrimidines are known to exhibit high structural diversity and complexity, as well as a wide range of physical, chemical, and biological properties. In this context, the present study aimed to propose new reaction conditions aligned with the principles of green chemistry, employing ionic liquids for the synthesis of tetrazolo[1,5-a]pyrimidine derivatives through a multicomponent reaction, a variant of the Biginelli reaction. The reaction conditions were optimized following a synthetic route catalyzed by PEI·IL, carried out under solvent-free conditions at 80 °C for 2 h, using 2 mmol of aldehyde**1**, 1 mmol of 5-aminotetrazole**2**and 1 mmol of ethyl acetoacetate or acetylacetone**3**(Scheme 1). Under these conditions, 18 tetrazolo[1,5-a]pyrimidine derivatives were successfully synthesized, with yields ranging from 8% to 96%. All products were fully characterized by HRMS, ^{1}H NMR, and ^{13}C{^{1}H} NMR spectroscopy.
The synthesized compounds were evaluated for their antimicrobial activity, showing minimum inhibitory concentration (MIC) values against Staphylococcus aureus (ATCC 25923) and Pseudomonas aeruginosa (ATCC 9027). Overall, this study demonstrates an efficient and sustainable methodology for the synthesis of tetrazolo[1,5-a]pyrimidines, fully consistent with green chemistry principles, notably through the absence of solvents and the use of a non-toxic catalyst.



Scheme 1. Synthesis of Tetrazolo[1,5-a]pyrimidine derivatives.

Agradecimentos/Acknowledgments

We are grateful to CAPES, CNPq, FINEP, FAPEG and UEG.

Benzophenone-Catalyzed Photoelectrochemical Dehydrogenative Cross-Coupling under Continuous Flow Conditions

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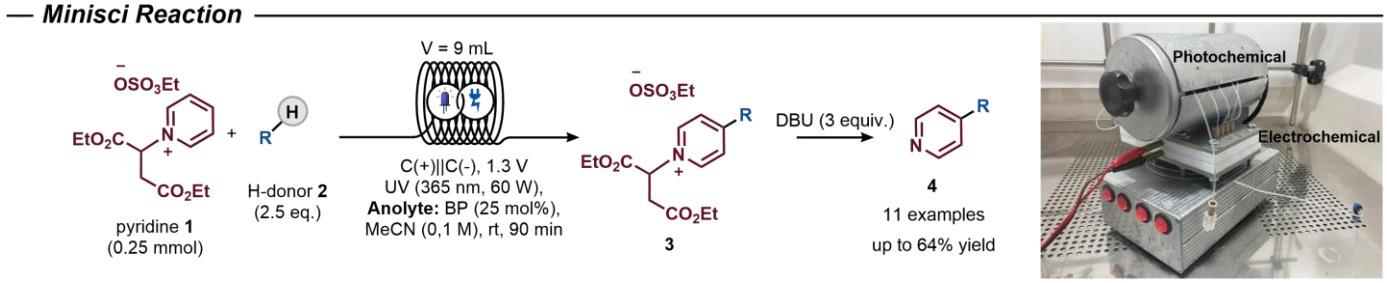
Palavras Chave:*Photoelectrocatalysis,Photochemistry,Electrochemistry,Continuous Flow,Benzophenone*

Highlights

We describe a continuous-flow photoelectrochemical reactor sustaining electrochemically mediated photoredox catalysis (e-PRC), enabling catalytic benzophenone without compromising performance.

Resumo/Abstract

Benzophenone (BP) is a well-established hydrogen atom transfer (HAT) photocatalyst, however, its broader synthetic utility is limited by rapid dimerization to benzopinacol under photochemical conditions. This off-cycle deactivation pathway prevents sustained catalyst turnover and typically requires stoichiometric amounts of BP.[1] Importantly, benzopinacol can be oxidatively cleaved under electrochemical conditions to regenerate benzophenone, providing a mechanistic basis for catalyst recycling.[2] In this context, electrochemically mediated photoredox (e-PRC) recycling represents a viable strategy to render benzophenone catalytically competent. Herein, we report a continuous-flow photoelectrochemical reactor that integrates light-driven HAT activation with electrochemical catalyst regeneration, enabling HAT photocatalysis with catalytic loadings of benzophenone. The synthetic utility of this platform was demonstrated in Minisci reactions between pyridine and alkyl partners, affording eleven examples of the desired products in yields of up to 64% using only 25 mol% BP, comparable to the 66% yield obtained under conventional stoichiometric conditions (150 mol%). This photoelectrochemical system was further applied to Paternò–Büchi cycloadditions and Giese-type alkylation reactions, which consistently delivered higher yields than purely photochemical approaches. Overall, these results demonstrate that continuous-flow recycling e-PRC effectively suppresses catalyst deactivation, expands reaction scope, and unlocks the catalytic potential of BP in HAT photocatalysis.



Minisci reaction enabled by a continuous-flow photoelectrochemical reactor.

Agradecimentos/Acknowledgments

The authors acknowledge FAPESP (RCS, 2023/07466-7 and 2025/02336-3; JCP, 2021/06661-5); CNPq (JCP, 301771/2025-1).

Bioprospecção de celulases produzidas por Bacillus spp. com potencial aplicação na biodegradação de resíduos orgânicos.

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Palavras Chave:*Bacillus spp., Celulases, Biodegradação, Vermelho Congo.*

Highlights

Screening of cellulase-producing*Bacillus*spp.;

Evaluation of the cellulolytic potential of bacterial strains;

Potential application in the biodegradation of organic waste.

Resumo/Abstract

Introdução: As celulases produzidas por*Bacillus*spp. são biocatalisadores eficientes devido à sua ação sinérgica enzimática (endoglucanases, exoglucanases e β-glucosidases) na hidrólise de celulose, apresentando alta especificidade e baixo custo energético. Com isso, este estudo teve o objetivo de explorar cepas de*Bacillus*spp. com potencial aplicação na biodegradação de resíduos orgânicos.**Metodologia**: Foram isoladas 20 cepas de*Bacillus*spp. de solos do município de Lagarto (SE) com reativação em Ágar Nutriente. As cepas viáveis foram submetidas a uma triagem celulósica em meio mínimo M9 com celulose microcristalina e teste com Vermelho Congo em Ágar Carboximetilcelulose, para obtenção do Índice Enzimático (IE). As cepas que apresentaram IE > 1,0 e viabilidade nos testes em placas, foram avaliadas em relação ao seu crescimento microbiano por Densidade Óptica (DO) em espectrofotômetro (600 nm).**Resultados e Discussão**: Das 20 cepas, 5 apresentaram crescimento no meio enriquecido com celulose microcristalina (1.1 B, 5 B, 7.1 A, 7.1 B e 10.1 A). No entanto, no teste do Vermelho Congo 11 cepas apresentaram IE > 1,0 (1.1 B, 2.1 A, 5 B, 6 A, 7.1 A, 7.1 B, 8 B, 10.1 A, 10 B, 12 B, 13.1 A). Foi medido o crescimento microbiano de 5 cepas (1.1 B, 5 B, 7.1 A, 7.1 B e 10.1 A), onde apenas 3 apresentaram crescimento ao longo das 96 horas. Após a curva de crescimento, as cepas 1.1 B, 7.1 B e 10.1 A mantiveram-se com DO_{600} acima de 0,100, apresentando valores de 0,221, 0,133 e 0,154, respectivamente, ao final das 96 horas.**Conclusão**: A partir da bioprospecção, obteve-se três cepas de*Bacillus*spp. (1.1 B, 7.1 B, 10.1 A) com potencial celulósico, que podem ser usados na biodegradação de resíduos orgânicos. Dessa forma, este estudo auxilia na busca de fontes alternativas que visam a otimização de processos agregando valor aos resíduos da agroindústria regional e promovam a química verde.

Agradecimentos/Acknowledgments

O autor agradece à Universidade Federal de Sergipe (UFS) e ao PROSGRAP pela concessão da bolsa, a orientadora Natália Nogueira Saraiva pelo acompanhamento científico e ao Laboratório de Química Geral e Orgânica (LaQuiGO) pela infraestrutura.

Bunte Salt Intermediates as a Platform for C-2 Sulfur-Functionalized Kojic Acid

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Palavras Chave:*Ácido Kójico,Sal de Bunte,Calcogênios.*

Highlights

Synthesis of C-2 chalcogen-functionalized kojic acid derivatives via Bunte salt intermediates and nucleophilic substitution of alkyl halides for biological evaluation.

Resumo/Abstract

Tyrosinase (TYR) is a key enzyme involved in melanin biosynthesis, a natural pigment responsible for protecting the skin against ultraviolet radiation. Dysregulation of TYR activity has been associated with hyperpigmentation disorders and skin cancer, highlighting the relevance of tyrosinase inhibitors in pharmacological research [1]. Kojic acid (KA) is widely recognized as a reference TYR inhibitor due to its ability to chelate copper ions in the enzyme's active site and is commonly used as a standard compound. Recent studies have shown that the incorporation of chalcogens, such as sulfur and selenium, into organic molecules can enhance biological activity, imparting antitumor and antioxidant properties [2-3]. However, reports on chalcogen introduction at the C-2 position of kojic acid remain scarce. In this context, this work investigates the C-2 functionalization of KA via Bunte salt intermediates, inspired by previously reported sulfur-transfer methodologies [4]. Additionally, KA was selectively protected at the C-5 hydroxyl group using a benzyl substituent in order to evaluate the influence of protection on molecular reactivity, which resulted in improved yields (87–96%, Fig. 1). The proposed approach enables access to sulfur-functionalized KA derivatives bearing aliphatic substituents, providing insights into their reactivity and supporting future biological evaluations.

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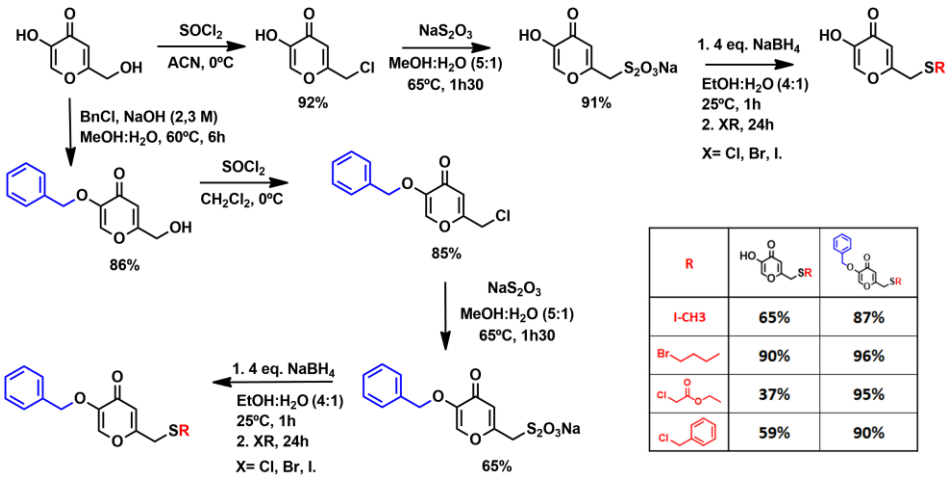


Fig. 1 - Methodology for C-2 sulfur-functionalization via Bunte salt intermediates and yields

Agradecimentos/Acknowledgments

CAPES, CNPq, UDESC, SINCA, FAPESC

C-3 Functionalization of the 4-Quinolone Core: Synthesis of Acylhydrazone Derivatives and Prospective Acyclonucleoside Analogues.

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Palavras Chave:*-Quinolones,Acylhydrazones,Acyclonucleosides,Antiviral agents,HIV-1 and HSV-1*

Highlights

C-3 functionalization of the 4-quinolone core afforded acylhydrazone derivatives with HIV-1 reverse transcriptase inhibition and enabled the synthesis of quinolone-based acyclonucleoside analogues.

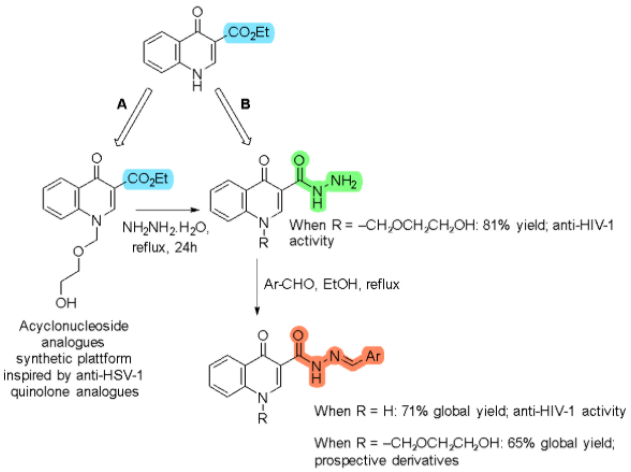
Resumo/Abstract

The 4-quinolone scaffold is widely recognized as a privileged structure in antiviral drug discovery, with functionalization at the C-3 position offering a versatile platform for molecular diversification. In this work, distinct synthetic strategies targeting the C-3 position of the 4-quinolone core were investigated, aiming at the development of structurally diverse derivatives with potential antiviral relevance. Initially, a series of C-3 acylhydrazone-substituted 4-quinolones was synthesized and evaluated as inhibitors of HIV-1 reverse transcriptase. These derivatives were obtained through reproducible synthetic protocols and exhibited significant enzymatic inhibition, with cytotoxicity profiles more favorable than that of zidovudine, in agreement with previously reported data. In parallel, quinolone-based acyclonucleoside derivatives were designed as structural analogues of nucleoside antivirals, inspired by the known anti-HSV-1 activity of related compounds. Although the biological evaluation of the acylhydrazone-containing acyclonucleosides is still ongoing, their synthesis was successfully achieved using established methodologies, enabling the incorporation of nucleoside-like moieties onto the quinolone framework. Taken together, the results highlight the C-3 position of the 4-quinolone nucleus as a strategic site for the introduction of functionally distinct groups, allowing the modulation of molecular properties relevant to antiviral activity. This study reinforces the versatility of the 4-quinolone scaffold and provides a solid synthetic foundation for future biological investigations of quinolone-based antiviral candidates targeting HIV-1 and HSV-1.

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C-3 functionalization of 4-quinolones yielding evaluated acylhydrazones and acyclonucleosides.

Agradecimentos/Acknowledgments

UFF, CAPES(fiance code 001), CNPq, FAPERJ.

Caracterização comparativa de resíduos do processamento do açaí

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Palavras Chave:*Biomassa de açaí;,Hidrólise ácida;,Caracterização química;,Elucidação estrutural.*

Highlights

Lignocellulosic structure of açaí residues.

Xylan-rich seeds; glucan-rich stalk and bunch.

Klason lignin and uronic acid evaluation.

Chemical platform for C5 and C6 valorization.

Resumo/Abstract

Aproveitar a biomassa do açaí, especialmente o caroço (que representa 80-85% do fruto), é importante por razões ambientais, econômicas, sociais e energéticas. No entanto, a valorização de materiais residuais de natureza orgânica requer a determinação precisa de sua composição química. Neste trabalho, três frações residuais do processamento do açaí — bastão, caroço e cacho — foram caracterizadas, com ênfase na fração polissacarídica e no teor de lignina. As amostras foram inicialmente submetidas à extração em Soxhlet com água e etanol, seguida da análise de lignina solúvel e insolúvel em ácido. A fração glicídica foi quantificada por cromatografia a líquido de alta eficiência em coluna catiônica, permitindo a determinação de açúcares estruturais e produtos de degradação. A determinação de lignina indicou diferenças estruturais entre as frações do processamento do açaí, evidenciando variações na proporção de material aromático associado à parede celular. As biomassas derivadas do bastão e do cacho apresentaram maiores teores de glucanas, enquanto o caroço destacou-se pelo elevado teor de polissacarídeos não estruturais. A presença de arabinose confirma a ocorrência de heteroxilanas nos materiais lignocelulósicos e a detecção de furfural nos hidrolisados de cacho e bastão confirmou essa observação. Conjuntamente, os resultados demonstram que as frações avaliadas apresentam organização lignocelulósica distinta, com implicações diretas no seu direcionamento a rotas de conversão química e bioquímica. Análises complementares encontram-se em desenvolvimento, incluindo composição elementar por CHNS-O, índice de cristalinidade por DRX, propriedades de superfície por XPS e caracterização da fração hemicelulósica por metanólise, incluindo a quantificação de ácidos urônicos. Tal abordagem permitirá estabelecer o perfil composicional comparativo entre as frações avaliadas, fornecendo subsídios para estabelecer o seu potencial no desenvolvimento de projetos de biorrefinaria.

Agradecimentos/Acknowledgments

Os autores agradecem à SBQ pela oportunidade de apresentação do trabalho, à UFPR pelo suporte institucional, ao orientador e grupo de pesquisa pelo apoio científico e ao CNPq pelo incentivo financeiro estudantil.

Carquejyl Acetate–Derived 1,3-Dicarbonyls as a Platform for the Biginelli Synthesis of Potentially Bioactive Dihydropyrimidinones

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Palavras Chave:*scaffold diversification,sustainable synthesis,1,3-dicarbonyl compounds,Biginelli reaction*

Highlights

Renewable carquejyl acetate was converted into diastereodivergent 1,3-dicarbonyls (52%, 48%) and then into Biginelli dihydropyrimidinones (6a 16%), with 6a under antitumor assays.

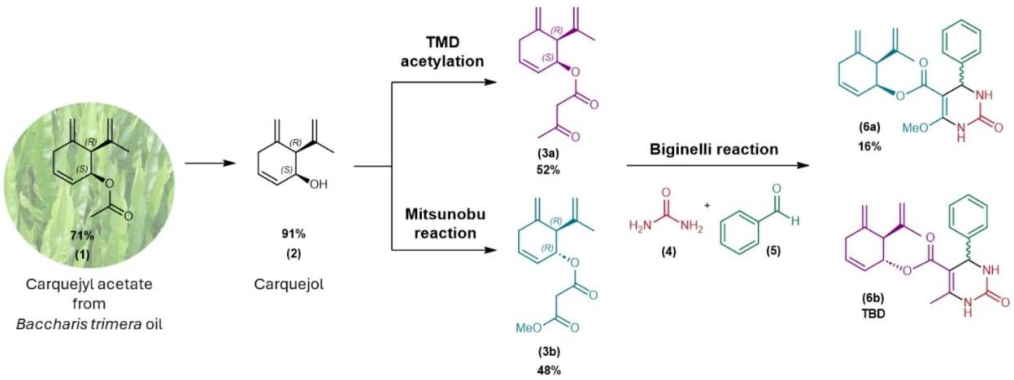
Resumo/Abstract

Baccharis trimera (carqueja) is a South American medicinal plant traditionally used for gastrointestinal, hepatic, and renal disorders and is included in Brazil's ReniSUS list of medicinal plants of interest. The essential oil of B. trimera is predominantly composed of carquejyl acetate (**1**) (~75%), accompanied by minor constituents such as the corresponding alcohol carquejol (**2**). First reported by Yves Naves in 1959 (2), carquejyl acetate remains a comparatively underexplored irregular monoterpene (rearranged monoterpene; ortho-menthane derivative), with limited stereochemical discussion in the literature (2,3). Motivated by its abundance, renewability, and local availability, we investigated carquejyl acetate as an enantiopure platform for scaffold generation. A series of transformations furnished two diastereomeric 1,3-dicarbonyl compounds,*syn*-(**3a**) and*anti*-(**3b**), in 52% and 48% yield, respectively. Diastereodivergence was achieved by tailoring the key stereochemical step:*syn*-(**3a**) was obtained via rapid acetylation using 2,2,6-Trimethyl-4*H*-1,3-dioxin-4-one (TMD), whereas*anti*-(**3b**) was accessed through a Mitsunobu protocol. Both 1,3-dicarbonyl derivatives were subsequently employed as β-dicarbonyl components in the Biginelli multicomponent reaction to afford dihydropyrimidinones (**6a**,**6b**), delivering structurally complex products (e.g.,**6a**isolated in 16% yield). Compounds**6a**is currently under biological evaluation for antitumor activity. Overall, this work highlights carquejyl acetate as a renewable, enantiopure terpene feedstock for the preparation of functionalized 1,3-dicarbonyl building blocks and their downstream diversification into dihydropyrimidinone scaffolds via Biginelli chemistry.

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Synthetic route from carquejyl acetate to dihydropyrimidinones.

Agradecimentos/Acknowledgments

The authors would like to thank Matologia Research Group at Universidade Federal do Paraná for donating the carqueja extract used in this work, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and Fundação Araucária for funding.

Cellulose Nanocrystals (CNCs) as dsRNA vectors for Gene Silencing in Sourgrass and Brown Stink Bug.

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Palavras Chave:*Nanocellulose, Gene Silencing, dsRNA, Nanocarrier, Cellulose Nanocrystals.,Nanocellulose,Gene Silencing,dsRNA,Nanocarrier,Cellulose Nanocrystals*

Highlights

Cellulose nanocrystals synthesized through hydrolysis and functionalized with betaine through esterification complexed dsRNA efficiently, inverting the charge and protecting dsRNA from degradation.

Resumo/Abstract

Gene Silencing mediated by interfering double-stranded RNA (dsRNA) is a natural mechanism in eukaryotic organisms and possesses a great potential for technological applications in weed and pest control. However, dsRNA molecules are hydrophilic, ionic and unstable, which makes it essential the development of delivery systems that provide cellular uptake and protection against enzymatic degradation. In this scenario, cellulose nanocrystals (CNCs) emerge as viable carriers, given their low toxicity, biocompatibility and flexibility to chemical surface modifications. This work has the objective to synthesize cellulose nanocrystals and to modify their surfaces to enable electrostatic complexation with dsRNA molecules.
CNCs were obtained by sulfuric acid-catalyzed hydrolysis of cotton fibers, resulting in nanocrystals with an average length of 197,91 ± 38,89 nm, an average surface charge of -25,29 ± 11,04 mV, and a yield of 16,30%, the analysis were done by DLS.
The esterification of CNCs was done by Steglich Method, resulting in inversion of surface charge to an average of +16,01 ± 8,39 mV and a yield of 70,88%, Infrared analysis indicated the existence of ester bands in 1748 cm^-1, confirming the success of the reaction.
The complexation was carried out using an aqueous solution of 2mg/ml of CNCs and two types of dsRNAs (dsRNA H for targeting of weed and dsRNA D for targeting of brown stink bug), at three concentrations (10, 50 and 100 ng/µl). In all cases, the complexation of the nanocrystals with dsRNA was observed to have been successful. Degradation assays were perfomed by incubating the complexed solutions with pure RNase and with RNase from the brown stink bug saliva for 15 minutes. Eletrophoretic analysis indicated partial protection in the case with the pure RNase and almost total protection in the case of the RNase from the bed bug saliva. Preliminary bioassays conducted with the target weed and beg bugs demonstrated effective delivery of dsRNA and Gene Silencing.

Agradecimentos/Acknowledgments

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Computational design of fluorescent BORANIL-based H2S probes

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Palavras Chave:*sensors,fluorescence,hydrogen sulfide,DFT*

Highlights

Quantum-chemical calculations support the use of fluorescent boranyl-based compounds as H_2S probes, revealing thermodynamic feasibility and reaction-induced photophysical changes.

Resumo/Abstract

Hydrogen sulfide (H_2S), is an endogenous gasotransmitter involved in essential physiological processes.[1] Its concentration in blood ranges from 10 to 100 µM, and abnormal levels are associated with diseases such as Alzheimer's, Parkinson's, and diabetes.[2] BORANIL complexes pose as an interesting alternative to BODYPY in the context of fluorescent H_2S probes, requiring fewer and simpler synthetic steps, utilizing commercially available precursors, and maintaining high quantum yields.[3] Despite these advantages, no fluorescent BORANIL-based fluorescent H_2S probes have been reported in literature. Herein, we present the first (TD)DFT investigation of the viability of BORANIL-derived compounds for H_2S sensing. Figure 1a presents the potential fluorescent probes, composed of dinitrophenyl (DNP) and BORANIL moieties connected through different linkers (**1a–c**). The DNP group, act as an efficient electrophile toward nucleophilic aromatic substitution (SNAr) with H_2S (Figure 1b), and as a fluorescent quencher via photoinduced electron transfer (PET).[4] Upon reaction, fluorescent compounds**2a–c**are released, rendering**1a–c**promising "*turn-on*" probes. Quantum-chemical calculations performed using ORCA 6.0 at the CAM-B3LYP/def2-TZVP level show that all reactions with H_2S are exergonic ($\Delta G<0$), indicating thermodynamic feasibility. Simulated photophysical properties reveal marked differences between probes**1a–c**and products**2a–c**. The absorption λ_{max} for**1a-b**are predicted 100–250nm range, whereas the fluorescence λ_{max} values**2a-b**, are close to 820 and 540 nm, respectively. The reaction mechanism is under investigation, by computing energy barriers and the characterization of Meisenheimer intermediates. The next stage includes synthesis and experimental photophysical evaluation of**1a–c**.

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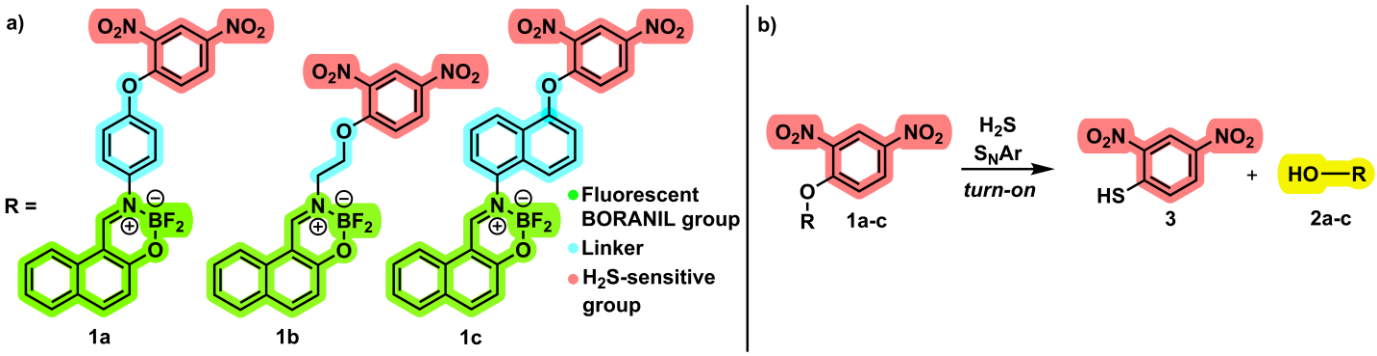


Figure 1: a) Structure of H2S probes 1a-c; b) Reaction between 1a-c and H2S forming compounds 2a-c .

Agradecimentos/Acknowledgments

To CAPES, CNPq and UFF.

Computational NMR of Fluorinated Aromatic Curcuminoids: Expanding ORCA Applications to Rigid Symmetric Systems

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Palavras Chave:*DFT,NMR Chemical Shift,fluorinated monoketonic curcuminoids*

Highlights

An accessible ORCA-based NMR and Chimera workflow using DFT calculations with scaling procedures showed good agreement with experimental ^{1}H and ^{13}C NMR chemical shifts in fluorinated aromatics.

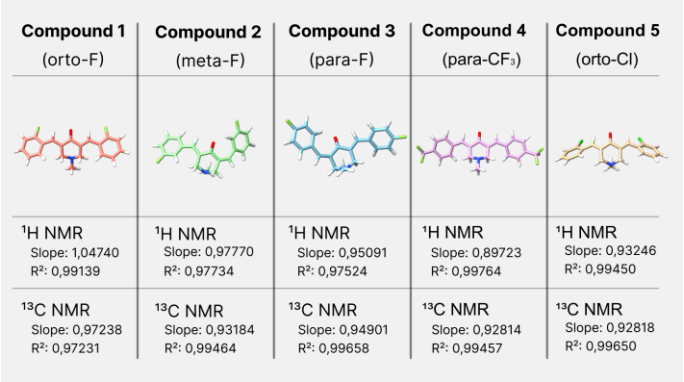
Resumo/Abstract

Although quantum chemical approaches have improved, accurate NMR chemical shift prediction in fluorinated systems remains method dependent, with deviations up to ~6.5 ppm for (hetero)aromatics and improved agreement for specific groups (RMSE ≈ 1.0 ppm for CF_3 and up to ~2.5 ppm for CF). Reliable predictions require accurate nuclear magnetic shielding tensors reflecting electronic charge distribution and magnetic anisotropy.

Monoketonic curcuminoids from*N*-methyl-4-piperidone were synthesized by Claisen–Schmidt condensation with substituted aromatic aldehydes, yielding fluorinated and CF_3 derivatives where the fluorine position modulated aromatic ^{1}H shifts: para substitution induced ortho shielding (+M), while meta substitution caused deshielding (–I) with multiplets at δH 7.41–7.37, 7.18–7.16 (J ≈ 7.8 Hz), and 7.09–7.06 ppm; ortho-chloro substitution caused pronounced ortho-proton deshielding consistent with chlorine's inductive effect.

DFT calculations were performed at the BP86/def2-TZVP(−f) level with def2/J, TightSCF, D3 dispersion, and CPCM (chloroform). NMR isotropic shieldings were computed using wB97M-V with the same basis set, and chemical shifts were obtained by scaling in ORCA 6.0 using conformational averages when relevant, reproducing experimental trends (Figure 1). For ^{13}C orto-Cl showed the best correlations (R^2 ≈ 0.996), while ^{1}H shifts correlated best for orto-Cl and CF3(R^2 ≈ 0.995–0.998); slopes below unity (^{1}H: ~0.90–0.98; ^{13}C: ~0.93–0.95) indicate systematic underestimation.

Whereas ORCA has been mainly applied to flexible and simple fluorinated systems, its consistent use here from conformational analysis to NMR calculations extends its applicability to rigid aromatic fluorinated compounds. Direct generation and visualization of NMR spectra from ORCA outputs in Chimera supports the reliability and accessibility of the adopted DFT protocol for NMR prediction and structural assignment.



Structures of compounds 1–5 and correlation of experimental and calculated ^{1}H and ^{13}C NMR shifts.

Agradecimentos/Acknowledgments

The authors thank CNPq, FAPESP, and FINEP for the continuous financial support and infrastructure provided to the NMR Laboratory.

Continuous Flow Hantzsch Ester–Enabled Photocatalytic Valorization of Lignin β-O-4 and Epoxy Resin Models

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Palavras Chave:*Biomass valorization,Lignin models,Photocatalysis,Hantzsch esters,Continuous flow*

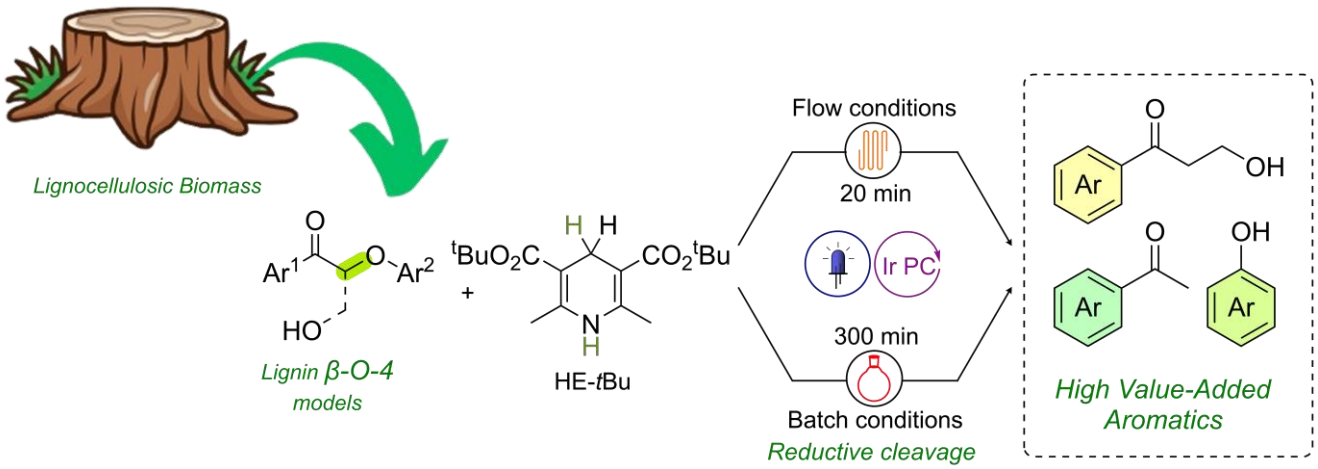
Highlights

Lignin and epoxy models were cleaved under blue light irradiation with an iridium-based photocatalyst with up to 91% isolated yield.

Transposition to flow regime shortened the reaction times.

Resumo/Abstract

Lignin is nature's most abundant source of aromatic compounds and constitutes an attractive renewable resource to produce aromatic commodity chemicals.Bearing this in mind, we disclose a continuous flow photocatalytic strategy for the valorization of oxidized lignin β-O-4 and epoxy resin model compounds. Using an iridium-based photocatalyst and Hantzsch esters as hydrogen donors, the method enables selective reductive C–O bond cleavage within 20 min, affording acetophenones and phenols as high value-added aromatic products in up to 91% yield. The protocol is readily extended to an oxidized epoxy resin model, enabling the formation of methylated bisphenol A and demonstrating its applicability beyond lignin-derived substrates. Collectively, these results establish a robust and scalable photoflow platform for the selective transformation of biomass- and polymer-derived C–O linkages.



Photocatalytic method for reductive cleavage reaction under batch versus flow conditions

Agradecimentos/Acknowledgments

The Authors acknowledge financial support from the São Paulo Research Foundation – FAPESP (PDB 2023/01232-4 and JCP, 2021/06661-5), and the Brazilian National Council for Scientific and Technological Development – CNPq (JCP, 301771/2025-1).

Continuous-Flow Manufacture of Rivaroxaban Intermediates via Chemo-Enzymatic approach

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Palavras Chave:*rivaroxaban,reduction,biocatalysis*

Highlights

Study of chemical and biotechnological reactions adapted to continuous-flow systems for the synthesis of rivaroxaban intermediates.

Resumo/Abstract

Rivaroxaban is an antithrombotic oxazolidinone that acts as a direct factor Xa inhibitor, used for the treatment of deep vein thrombosis.[1] Developed by Bayer AG (Xarelto®), its synthesis presents challenges such as low yields and unsatisfactory enantiomeric ratios in key intermediates, such as 4-(4-aminophenyl)morpholin-3-one (37% yield) and (*S*)-glycidyl phthalimide (E = 44 in 20 h).[2] In this context, adaptation to continuous-flow systems offers significant advantages regarding efficiency and reaction control.

To optimize the synthesis of rivaroxaban intermediates using chemical and biotechnological strategies under continuous-flow conditions.

The synthesis of 4-(4-aminophenyl)morpholin-3-one was investigated via catalytic hydrogenation and $Na_2S_2O_4$ reduction in tube-in-tube, H-Cube, and Chemtrix reactors. The enzymatic kinetic resolution of (*S*)-glycidyl phthalimide was performed with Lipase PS from Burkholderia cepacia immobilized in a fixed-bed reactor. Conversion, selectivity, and enantiomeric excess were determined by HPLC-DAD, with product identification by IR and ^{1}H and ^{13}C NMR.

Hydrogenation in a tube-in-tube reactor achieved >99 conversion and 84% selectivity (7 min at 80 °C). In the H-Cube system, the time was reduced to 24 s, with 73 conversion and 27% selectivity. The best results were obtained with $Na_2S_2O_4$ in a Chemtrix reactor, reaching >99% conversion and selectivity in 20 min. In the enzymatic resolution, optimized batch conditions provided an enantiomeric ratio (E) >200 (ee = 96%) in 8 h. Under continuous-flow (fixed-bed), 44% conversion was obtained in 30 min (eep = 89%; E = 46).

The study demonstrates the feasibility of continuous flow in rivaroxaban synthesis. The $Na_2S_2O_4$ reduction was highly efficient, and the enzymatic route improved enantioselectivity, although further optimizations are required to increase E values under flow conditions.

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Agradecimentos/Acknowledgments

The authors thank the Institute of Chemistry of the Federal University of Rio de Janeiro (IQ-UFRJ) and the funding agencies CNPq and CAPES for financing the research.

Continuous flow synthesis of Dolutegravir via acyl ketenes chemistry.

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Palavras Chave:*Integrase inhibitor,acyl ketenes,HIV.,HIV*

Highlights

An alternative approach is being developed by telescoping intermediates via acylketenes to afford dolutegravir under continuous flow conditions.

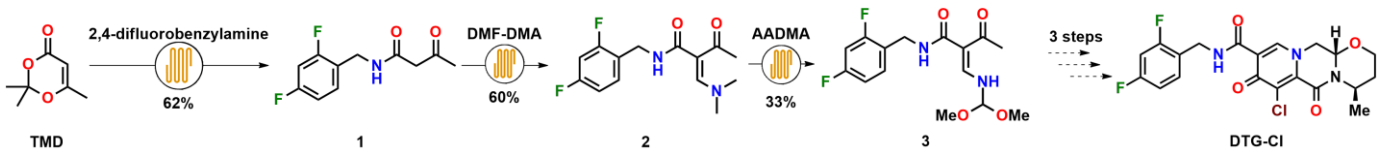
Resumo/Abstract

Since the introduction of raltegravir in 2007, several structural analogues have been developed, notably dolutegravir (DTG). DTG is considered an essential medicine by the World Health Organization (WHO) and extensively used in HIV therapy.[1] In the literature, the synthesis of dolutegravir has been reported under both batch and continuous-flow conditions. In 2008, described an efficient semi-telescoped flow approach, affording the desired compound in seven steps with an overall yield of 24%.[2] However, this route relies on an expensive β-keto ester as the starting material, potentially limiting scalability, and requires high temperatures to access the amide moiety. An alternative strategy to access β-keto esters or amides involves the use of 2,2,6-trimethyl-4*H*-1,3-dioxin-4-one (TMD), which generates ketenes*in situ*under thermal conditions, as previously demonstrated by our group.[3] On this basis, we are developing a seven-step synthetic pathway in which the amide is accessed under milder conditions using an accessible reagent (TMD). In this route, the amide (**1**) moiety is introduced in the first step, affording 62% yield. Subsequent transformation using DMF–DMA provided the corresponding intermediate (**2**) in 60% yield. The third step has been successfully achieved with a preliminary yield of 33% (**3**), and optimization studies are currently ongoing. In parallel, a semi-telescoped continuous-flow route to DTG-Cl via TMD-derived acylketene intermediates is under development.

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1. General scheme starting from TMD to afford DTG.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge financial support from the São Paulo Research Foundation – FAPESP (LCF 2024/22317-0 and JCP 2021/06661-5), the Brazilian National Council for Scientific and Technological Development – CNPq (JCP, 301771/2025-1)

Demethylation of guaiacol using a divided electrochemical cell

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Palavras Chave:*Organic synthesis, Electrochemistry.*

Highlights

The demethylation of guaiacol generating catechol, performed in an undivided cell using electrodes of magnesium and stainless steel in the presence of LiBr, dimethylurea and TPPA in THF.

Resumo/Abstract

The environmental impact caused by the extensive use of fossil fuels has driven the search for more sustainable and alternative technologies, that utilize renewable energy sources and biomass derivatives as substrates to produce the same industrial commodities produced from the petroleum matrix. In this work, we present the demethylation of guaiacol, derived from the abundant aromatic natural polymer lignin[1], to produce catechol, used in the chemical industry as raw material for the synthesis of perfumes, drugs, pesticides and dyes[2]. The reaction occurs in an undivided electrochemical cell with a galvanostatic condition using electrodes of magnesium and stainless steel as anode and cathode, respectively. In the presence of tris(pyrrolidino)phosphoramide (TPPA), a stabilizer for the solid ewlectrolyte interphase (SEI) formed on the electrodes during the reaction, LiBr as support electrolyte and dimethylurea as proton donor[3], the reaction yielded 41% of the product. The screening of the reaction conditions is in progress and will be presented. References: 1) SUN, Zhuohua et al. Bright side of lignin depolymerization: toward new platform chemicals.**Chemical reviews**, v. 118, n. 2, p. 614-678, 2018. 2) FIEGE, Helmut et al. Phenol derivatives.**Ullmann's encyclopedia of industrial chemistry**, 2000. 3) PETERS, Byron K. et al. Scalable and safe synthetic organic electroreduction inspired by Li-ion battery chemistry.**Science**, v. 363, n. 6429, p. 838-845, 2019.

Entry	Solvent	Electrodes	F (mol e^-/mol)	Yield of catechol (%)[a]
1	THF (0.06 M; 4 mL)	Mg(+)|SSW (-)	7.7	41
2	THF (0.06 M; 6 mL)	Mg(+)|SSW(-)	7.7	11
3	THF (0.06 M; 4 mL)	Mg(+)|SS(-)	7.7	12
4	THF(0.03 M; 6 mL)	Mg(+)|SS(-)	9	30
5	THF (0.06 M; 6 mL)	Mg(+)|SS(-)	6.2	16[b]

Table 1. Experiments conditions of the demethylation of guaiacol.

Agradecimentos/Acknowledgments

The authors acknowledge financial support from São Paulo Research Foundation–FAPESP (LGR, 2024/18522-8; RCS, 2025/02336-3; JCP, 2021/06661-5) and the Brazilian National Council for Scientific and Technological Development – CNPq (JCP, 301771/2025-1).

Desenvolvimento de metodologia verde, one-pot, solventless de Imidazo[1,2-a] piridinas utilizando Ácido Tribromoisocianúrico (TBCA)

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Palavras Chave:*2-a] pyridines One-pot synthesis; Green Chemistry,2-a] pyridines; One-pot synthesis; Green Chemistry,Imidazo[1.2-a] pyridines,One-pot synthesis,Green Chemistry*

Highlights

Development of new green methodology to synthesize imidazo[1,2-a] pyridines under solvent-free conditions using tribromoisocyanuric acid as halogenation reagent.

Resumo/Abstract

O núcleo heterocíclico imidazo[1.2a] piridinas são bastante cobiçados por sua mais diversas atividades biológicas como antivirais, antibacterianos, antifúngicos e anti-inflamatório. 1 A utilização de condições reacionais mais brandas e que atendam às exigências dos princípios da química verde são imperativos importantes em uma realidade cada dia mais preocupada com questões ambientais.2 Reações sem solvente, ou em solventes verdes, e que utilizem reagentes que possam ser recuperados em outro momento apresentam um importante grau de verdura e agregam importante valor a síntese de compostos de interesse medicinal. Este trabalho tem como principal objetivo desenvolver metodologia de síntese imidazo[1,2-a] piridinas a partir de derivados 2-aminopiridinas, compostos carbonilados alquil-aril-cetonas e o uso do ácido tribromoisocianúrico (TBCA) como agente de halogenação. Nosso melhor resultado foi obtido a partir da reação entre 1,1 mmol de acetofenona, 1,0 mmol de TBCA, 1,0 mmol de 2-aminopiridina, 2,0 mmol de trietilamina, sem solvente, à 60ºC - 65ºC em 24 horas de reação sob sistema de refluxo, obtendo, após a etapa de purificação e isolamento com coluna cromatográfica, o produto em rendimento de 21%. Este trabalho continua sob investigação das condições reacionais como temperatura, condições de micro-ondas, mudança da base e outros parâmetros, a fim de obter melhor rendimento na obtenção do produto imidazo[1,2-a] piridinas.

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2-Lenardão, E. J., Freitag, R. A., Dabdoub, M. J. et al. Química Nova 2003 26, 123

Agradecimentos/Acknowledgments

We would like to thank the Instituto Multidisciplinar de Química, Centro Multidisciplinar UFRJ-Macaé.

Design and Synthesis of Triazino[5,6-b]indole-Menadione Hybrids as Promising Multitarget Anticancer Agents

Isadora Maria Gouveia Andrade (PG)*[1], Mariana de Oliveira Leal Desmarais (IC)[1], Caio Luiz Festas Valadão (IC)[1], Edson de Oliveira Lima Filho (PQ)[1], Vitor Francisco Ferreira (PQ)[1], Luana da Silva Magalhães Forezi (PQ)[1], Fernando de Carvalho da Silva (PQ)[1].

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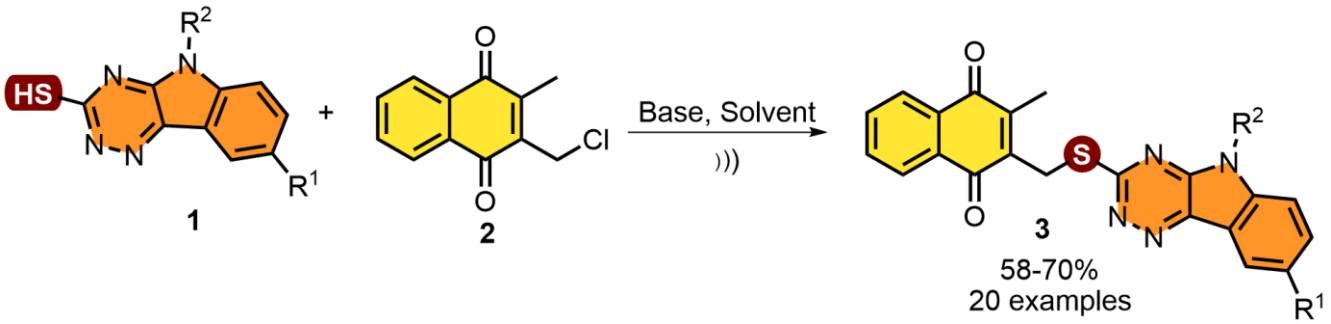
Palavras Chave:*Drug resistance, Small-molecule library, Vitamin K derivatives, Antiproliferative activity, Medicinal chemistry*

Highlights

Molecular hybridization is a powerful strategy for multitarget anticancer design. Triazinoindole and menadione scaffolds show promising antiproliferative potential.

Resumo/Abstract

Cancer remains one of the leading causes of global mortality, being characterized by high molecular complexity, toxicity associated with conventional therapies, and the frequent development of therapeutic resistance.[1] In this context, the discovery of new anticancer agents with a multitarget profile has emerged as a promising strategy in medicinal chemistry.[1] Molecular hybridization represents a rational approach for integrating different bioactive pharmacophores into a single chemical entity, potentially leading to compounds with improved efficacy and selectivity.[1–3]The indole ring is widely recognized as a privileged scaffold in medicinal chemistry, whereas fused triazino[5,6-*b*]indole**1**systems have demonstrated relevant anticancer and antiproliferative activities, as well as the ability to modulate multiple cellular pathways.[1] Menadione (vitamin K_3)**2**, in turn, exhibits well-documented anticancer activity, mainly associated with apoptosis induction and cell cycle modulation.[4] In this work, we describe the design and synthesis of a new series of triazino[5,6-*b*]indole-menadione hybrids**3**obtained through direct conjugation of the**1**core to**2**via SN_2-type reactions. The synthetic protocol proved to be efficient, affording the target hybrids in 58-70% yields (**Scheme 1**) and enabling the rapid generation of a novel compound library. The triazino[5,6-*b*]indole core was prepared from isatin according to previously reported procedures. The adopted strategy aims to integrate, within a single molecular framework, pharmacophores capable of simultaneously acting on multiple targets involved in tumor progression. The synthesized compounds will be forwarded for biological evaluation in order to assess their antiproliferative and anticancer potential. [1] Badawi, A.; et. al.*Bioor. Chem.*, 2025, 165, 108943;[2] Patel, V.; et al.*ACS Chem. N.*, 2019, 10, 3635-3661; Tamaddon-Abibigloo, Y .et al.*Bioor. Chem.*, 2024, 147, 107355; [4] Abdassalam, A. F. S. et al.*M. Chem.*, 2023, 32, 484.



Scheme 1. Synthetic route for the new series of triazino[5,6-b]indole-menadione hybrids.

Agradecimentos/Acknowledgments

CNPq, CAPES, PPGQ-UFF.

Development of 2,4,6-triphenylpyridine-based luminescent discotic liquid crystals via the Hantzsch methodology.

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Palavras Chave:*Liquid Crystals, Pyridine, Hantzsch Synthesis, Luminescence, Organic Synthesis*

Highlights

Synthesis of pyridine-derived luminescent discotic liquid crystals via the Hantzsch methodology for application in organic electronics.

Resumo/Abstract

Luminescent discotic liquid crystals have recently attracted significant attention due to their potential to revolutionize the Organic Light-Emitting Diodes (OLEDs) industry, as their self-organization and anisotropic emission can significantly enhance device efficiency. However, practical applications require efficient luminescence and room temperature liquid-crystalline behavior, which can be favored by reducing molecular symmetry [1]. For this purpose, a better understanding of the impact of structural modifications is required. Thus, five structures derived from the 2,4,6-triphenylpyridine core were designed using the Hantzsch multicomponent methodology [2], an efficient approach for the synthesis of less symmetrical pyridines. The molecules were conceived with different numbers and positions of aliphatic chains, aiming at symmetry reduction, and allowing the evaluation of the impact of these modifications on their photophysical, and liquid-crystalline properties. Moreover, comparison with analogous molecules containing benzene or 1,3,5-triazine as the central unit enables assessment of the influence of the pyridine ring on the material properties, as the presence of nitrogen atoms reduces steric hindrance and promotes greater structural planarity, influencing its properties. The proposed molecules (Fig.1a) were successfully synthesized and characterized. Absorption and emission spectroscopy studies in the UV–Vis region revealed luminescent behavior, with emissions between 313 and 395 nm. Among the analyzed structures, molecule N-322, bearing seven long aliphatic chains, exhibited columnar mesomorphism in the temperature range of 30–50 °C (Fig. 1b). This behavior represents a favorable indication of the application potential of these molecules and motivates the expansion of the structural scope proposed in this project.

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[2] Medeiros, J. V. S.*et al*.,*Dyes and Pigm.,*230, 112361 (2024).

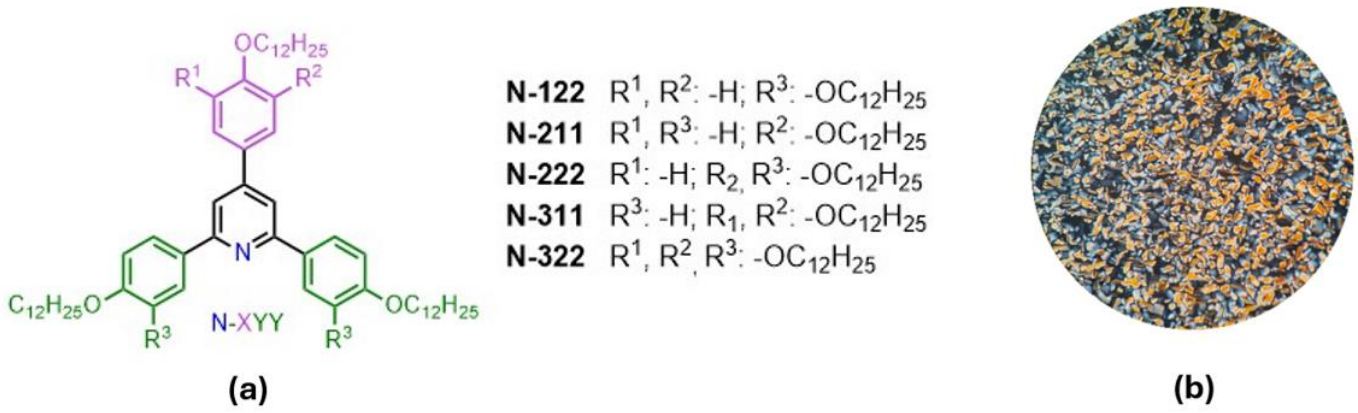


Figure 1. (a) General representation of the five studied molecules; (b) Mesophase texture of N-322.

Agradecimentos/Acknowledgments

UFSC, PPGQ, CNPq, CAPES, INCT-INEO, FAPESC.

Development of a new solvent-free mechanochemical N-arylation of 4-chloroquinolines

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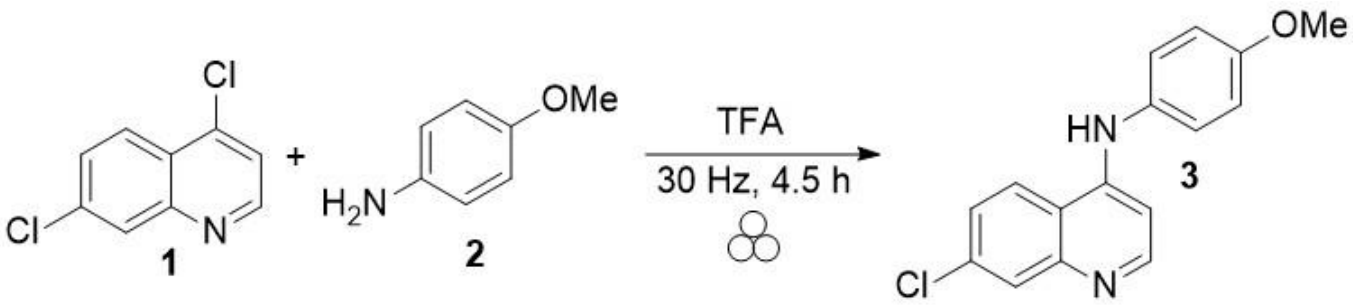
Palavras Chave:*4-Anilinoquinolines,Antimalarial compounds,Mechanochemistry,,Mechanochemistry,Sustainable methodologies*

Highlights

Due to the antimalarial potential of quinoline compounds, in this work we are investigating more sustainable methodologies to synthesize these scaffolds using mechanochemical approaches.

Resumo/Abstract

4-aminoquinolines are considered privileged scaffolds in medicinal chemistry, since their structure can be observed in several compounds with anticancer, antifungal, antileishmanial, anti-inflammatory, antianalgesic, anti-Alzheimer, and antimalarial activities.[1] In order to develop a more sustainable synthetic methodology to synthesize 4-anilinoquinolines from 4-chloroquinoline, in this work, we are studying a new SNAr reaction under mechanochemical conditions. Thus, to achieve the best condition for performing the*N*-arylation reaction, we chose 4,7-dichloroquinoline (**1**) and*p*-anisidine (**2**) as standard substrates (Scheme 1). In sequence, some solvent-free tests were evaluated by varying parameters such as milling frequency, reaction time and catalysts. After many tests, we may achieve full conversion (GC-FID) of 4,7-dichloroquinoline (**1**) to the 7-chloro-*N*-(4-methoxyphenyl)quinolin-4-amine (**3**) using TFA as catalyst, a milling frequency of 30 Hz for 4.5 h at 25 °C, resulting in 98% isolated yield. Subsequently, we applied this methodology using*o*-anisidine, which allowed us to obtain the respective 4-anilinoquinoline in 53% yield. Although the lower yield can be attributed to steric hindrance exerted by the methoxy group at the*ortho*-position, we intend to evaluate minor modifications to the methodology to improve this yield. In summary, we developed a new solvent-free*N*-arylation methodology via mechanochemistry, which was able to provide two 4-anilinoquinolines (**3**) in moderate to good yields, demonstrating the potential of mechanochemistry for the sustainable synthesis of heterocyclic compounds. Moreover, further studies aimed at exploring the scope of the methodology and obtaining a variety of 4-anilinoquinolines are currently being investigated in our research group.
[1]Delgado, F.; Benítez, A.; Gotopo, L.; Romero, A. H.*Front. Chem.***2025**,*13*, 1553975



Scheme 1

Agradecimentos/Acknowledgments

CNPq, FACEPE and iCEIS.

Development of a Sustainable Route for the Synthesis of Furoic Esters and Amides via Steglich Esterification

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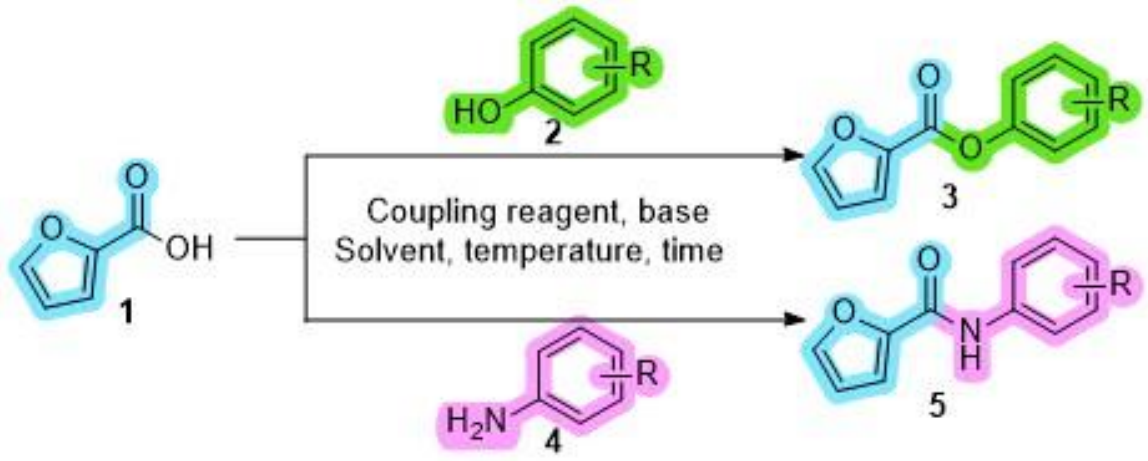
Palavras Chave:*Steglich esterification,4-hydroxyphenylpyruvate dioxygenase,HPPD,Enzymatic inhibition,green chemistry*

Highlights

Anisole proved an excellent green solvent for furoic ester and amide synthesis, replacing acetonitrile and DCM. Over 20 compounds were obtained with moderate to excellent yields.

Resumo/Abstract

Steglich esterification is a widely used methodology for the synthesis of esters and amides, allowing the efficient conversion of carboxylic acids under mild conditions through the use of a coupling agent and an organocatalyst at room temperature. Despite its synthetic efficiency and broad functional group tolerance, conventional protocols present limitations regarding sustainability. In this context, this work investigates Steglich esterification guided by Green Chemistry principles, focusing on the selection of lower environmental impact solvents and renewable feedstocks. Sustainable solvent selection guides recommend replacing chlorinated solvents with less toxic alternatives, including aromatic ethers and solvents derived from renewable sources. Additionally, the use of biomass-derived substrates, such as renewable carboxylic acids, contributes to improving the overall sustainability of the process. Accordingly, the adaptation of Steglich esterification for the synthesis of functionalized furoic acid derivatives emerges as a promising strategy, combining synthetic efficiency and environmental responsibility. This methodology enabled more sustainable substitutions in the synthesis of 25 herbicide candidate compounds, with yields ranging from 24 to 82%, currently under biological evaluation. Preliminary results indicate favorable performance compared to the reference compound, highlighting the potential of this approach for the development of safer and more efficient molecules. All products were fully characterized by spectroscopic techniques. References: [1] ANASTAS, P. T.; WARNER, J. C. Oxford University Press, 2000. [2] BYRNE et al. Sustainable Chemical Processes, 2016, 4(1), 1–24. [3] JORDAN, A.; WHYMARK, K. D.; SNEDDON, H. F. Green Chemistry, 2021, 23, 6405–6413.



Scheme 1. General synthetic route towards furoic esters and amides.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge FAPERJ, CNPq and CAPES for funding, as well as PPGQ-UFF.

Development of New C6-functionalized Coumarin-Benzothiazoles: Synthesis and Photophysical Properties.

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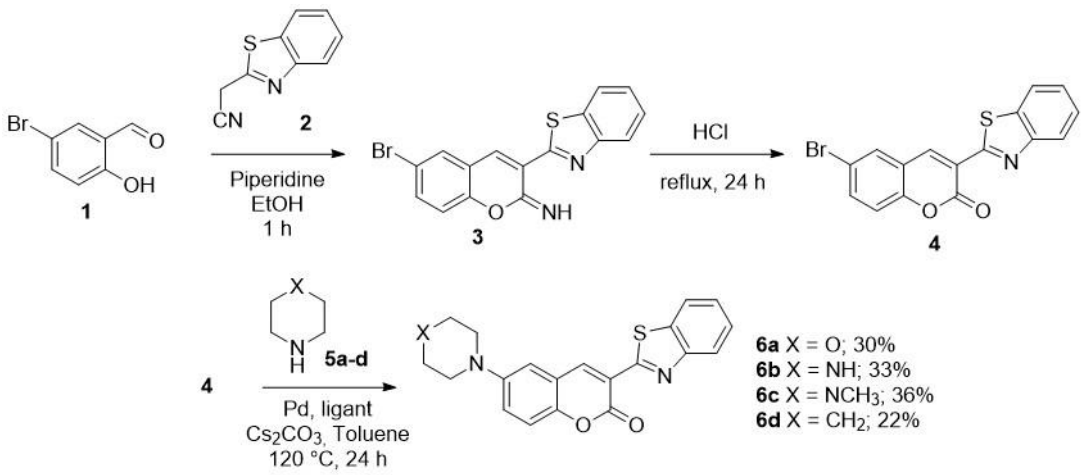
Palavras Chave:*fluorophore, heterocycle, optical properties.,fluorophore,heterocycle,optical properties*

Highlights

Coumarin-benzothiazole hybrids were successfully synthesized with moderate yields. Their photophysical properties were evaluated in different solvents.

Resumo/Abstract

Fluorophores play a central role in modern chemical analysis and related fields, as fluorescence is one of the most sensitive and informative techniques available. As a result, continuous research efforts have focused on the development of new organic fluorescent materials with tunable optical properties. Among the various classes of organic fluorophores, coumarin derivatives stand out due to their strong absorption in the ultraviolet–visible region, high fluorescence quantum yields, structural versatility, and good biocompatibility, which make them attractive for a wide range of fluorescence-based applications. In this work, a series of novel coumarin–benzothiazole derivatives (**6a–d**) was synthesized through a multistep synthetic route starting from an iminocoumarin precursor. The benzothiazole**2**intermediate was initially obtained via a cyclization reaction between*o*-aminothiophenol and malononitrile, followed by condensation with 5-bromo-2-hydroxybenzaldehyde**1**under piperidine catalysis to afford an iminocoumarin–benzothiazole intermediate**3**. This intermediate was subsequently converted into the corresponding coumarin**4**under acidic conditions. The final compounds**6a-d**were obtained after optimization of Buchwald–Hartwig cross-coupling reactions, employing XPhos Pd G2 (17 mol%) and XPhos (2 mol%), leading to moderate isolated yields (22-36%). Photophysical properties of the synthesized compounds were investigated using UV–Vis absorption spectroscopy. The absorption spectra exhibited intense bands in the UV to green region, with maximum absorption wavelengths (λ_max) ranging from 350 to 355 nm and high molar absorptivities (ε) on the order of 10^4 L mol^{-1} cm^{-1}, indicating efficient electronic transitions. The optical band gap energies, estimated from the absorption onset, were found to be in the 2,46–2,57 eV range, highlighting the influence of molecular structure on the electronic properties of the coumarin–benzothiazole systems.



Scheme 1. Synthesis of C6-functionalized Coumarin-Benzothiazoles 6a-d.

Agradecimentos/Acknowledgments

FAPERJ, CNPq, CAPES, and FIOCRUZ

Development of new Docusate-Based Ionic Liquids: Synthesis, Characterization, and Thermal Properties

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Palavras Chave:*ionic liquids,Docusate-Based*

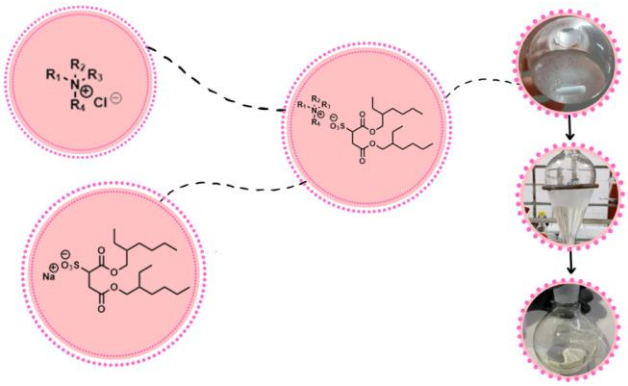
Highlights

Four docusate-based ionic liquids were synthesized and characterized. Docusate is reinforced as a promising anion for more sustainable solvents.

Resumo/Abstract

Ionic liquids (ILs) have emerged as environmentally and sustainably solvents due to their properties such as low vapor pressure, high thermal and chemical stability, low volatility, and recyclability. With the possibility of cation and anion modulation, the anionic surfactant sodium docusate offers a rapidly biodegradable, negligible volatility, and low-cost alternative.[1] From this perspective, the present work demonstrates the synthesis and characterization of ILs based on the sodium docusate anion. Four ionic liquids [BZT][DC], [BZK][DC], [EHD][DC], and [DAB][DC] were prepared in acetone/water (1:1), followed by liquid-liquid extraction with distilled water. After obtaining the solvents, they were characterized by infrared (IR), NMR, TGA, and DSC. The synthesized ionic liquids were obtained after 15-19 hours of reaction and exhibited viscous, colorless liquid characteristics, with no crystallization at room temperature, indicating the efficiency of the synthetic route employed. Infrared spectroscopy analyses confirmed the formation of ionic liquids through the presence of characteristic bands of the docusate anion, as well as the functional groups associated with the respective cations. 1H and 13C NMR spectra confirmed the proposed structures, with no relevant impurities observed, and TGA analyses demonstrated high thermal stability of the obtained ionic liquids. The results obtained demonstrate that the employed methodology was effective for the synthesis of ionic liquids based on the sodium docusate anion, yielding materials with high purity, thermal stability, and properties characteristic of ionic liquids. Thus, the synthesized ILs show promise as alternative solvents with reduced environmental impact, reinforcing the potential of the docusate anion in developing more sustainable ionic liquids, owing to its biodegradability and low toxicity.

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Synthesis of ionic liquids

Agradecimentos/Acknowledgments

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Development of Novel Coumarin-1,2,3-Triazole Hybrids via Amide Coupling as Potential Theranostic Agents for Alzheimer's Disease

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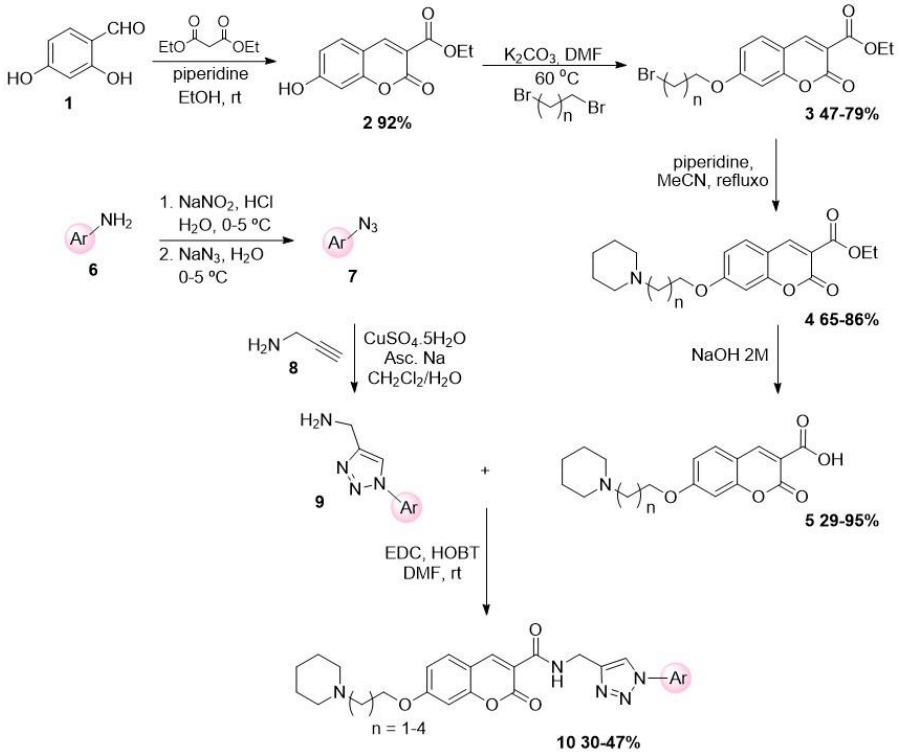
Palavras Chave:*Theranostic Agents,Neurodegenerative Diseases,Cholinesterases inhibitors,β-Amyloid Aggregation,Heterocycles*

Highlights

Novel coumarin-1,2,3-triazole hybrids were synthesized via EDC/HOBt-mediated amide coupling. The compounds are being evaluated as multifunctional theranostic agents for Alzheimer's disease.

Resumo/Abstract

The search for new drugs capable of reducing or eliminating the morbidity and mortality rates of patients affected by various diseases has been one of the main focuses of organic synthesis associated with medicinal chemistry. Among these diseases are neurodegenerative diseases, which are pathologies characterized by the progressive death of neurons, being one of the leading causes of dementia worldwide. Alzheimer's disease (AD) is considered the most common form of dementia.[1] The understanding of AD disorders led to the development of new medications, such as cholinesterase inhibitors, inhibitors of proteins such as β-amyloid peptide (Aβ) and metal chelating agents.[2,3] In addition, Theranostic agents capable of simultaneously detecting and inhibiting Aβ plaques are crucial for early AD management. In this context, Coumarins represent a privileged scaffold for this purpose due to their biological versatility and fluorescence properties, acting as potential probes for diagnosis and therapy for AD.[4] In this work, novel coumarin-1,2,3-triazole hybrids were synthesized via an EDC/HOBt-mediated amide coupling. These compounds were obtained in satisfactory yields and are currently under investigation for their inhibitory activity against acetylcholinesterase and β-amyloid aggregation, as well as their metal chelating properties aiming at the diagnosis and treatment for AD.



Scheme 1. Synthesis of coumarin-1,2,3-triazole hybrids.

Agradecimentos/Acknowledgments

CAPES, CNPq, and FAPERJ.

Development of smart bandages based on sodium alginate and red cabbageanthocyanins

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Palavras Chave:*Smart Bandages, Sodium Alginate, Anthocyanins.,Smart Bandages, Sodium Alginate, Anthocyanins*

Highlights

Smart bandages for wound pH monitoring. Alginate–anthocyanin system. Covalent pigment binding improves stability and colorimetric response.

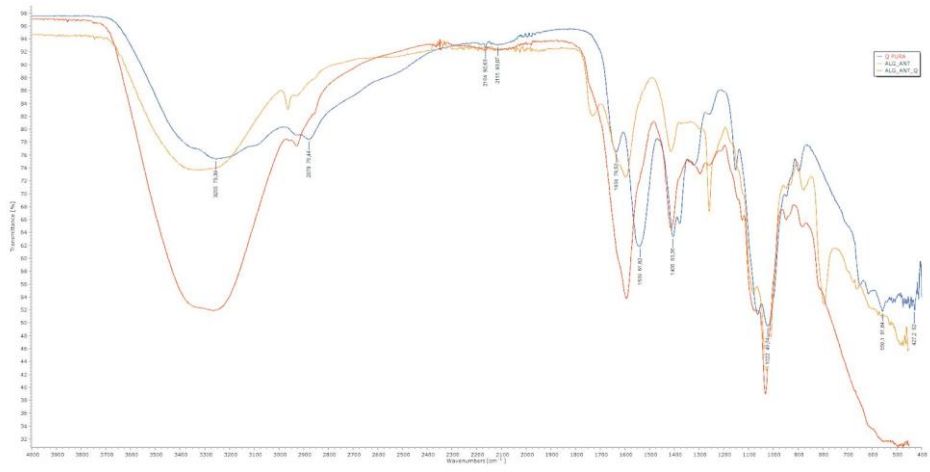
Resumo/Abstract

Chronic wounds represent a major healthcare challenge, and real-time monitoring of their healing process is essential for improving patient outcomes. This study presents the development of smart bandages capable of detecting pH variations, a key indicator of wound infection. The system is based on anthocyanins, natural pH-sensitive pigments, combined with sodium alginate, a biopolymer widely used in wound dressing applications.

The main innovation of this work lies in the covalent bonding of anthocyanins to alginate, aiming to overcome the inherent instability of these pigments. Anthocyanins were extracted and concentrated from red cabbage, and alginate modification was carried out using either EDC/NHS coupling chemistry or protic acid catalysis. After dialysis to remove non-bound pigments, samples prepared with concentrated extract under acidic conditions exhibited intense and stable coloration, suggesting successful covalent attachment.

FTIR analysis confirmed the formation of new chemical bonds, including ester groups, indicated by band broadening around 1600 cm^{-1}. Crosslinking strategies were evaluated to improve moisture resistance. Calcium chloride crosslinking was ineffective, likely due to the consumption of alginate carboxylate groups during pigment binding. In contrast, chitosan crosslinking produced thicker gels and enhanced colorimetric response over a range of pH values. Additional studies are underway to clarify the role of chitosan, and stabilizing agents such as ascorbic acid are being investigated to further improve pigment stability.

These results demonstrate that covalent bonding between anthocyanins and alginate is feasible and yields a material with promising colorimetric properties for pH sensing in wound environments. Further optimization is required to obtain a commercially viable smart bandage.



FTIR spectra comparing chitosan, alginate + anthocyanin and alginate + anthocyanin + chitosan

Agradecimentos/Acknowledgments

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Diastereoselective Mannich Synthesis of 2-(Anilino(phenyl)methyl)cyclohexan-1-one Catalyzed by Mixed-Phase Magnesium and Bismuth Species

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Palavras Chave:*Mannich Reaction,Heterogeneous catalyst,Diastereoselectivity,Bismuth*

Highlights

MgBi catalysts were evaluated in the Mannich reaction.

Conversions above 99% and na 82:17*anti/syn*ratio were achieved.

Resumo/Abstract

The Mannich reaction is a multicomponent reaction (MCR) characterized by a one-pot combination of a primary or secondary amine, an aldehyde, and a ketone [1]. Diastereoselective control in MCRs remains a significant challenge in organic synthesis, particularly when the simultaneous formation of new stereogenic centers is involved [2]. In this context, the Mannich reaction stands out as a versatile tool for the synthesis of structurally complex β-aminocarbonyl compounds, whose formation often involves multiple stereogenic centers, making diastereoselectivity control essential in the synthetic process [3]. In this work, catalysts were synthesized as mixed-phase systems containing bismuth and magnesium species (MgBi) and compared with catalysts composed solely of mixed-phases magnesium species or exclusively of bismuth species [4]. They were applied to control the diastereoselectivity of the reaction between cyclohexanone (1 mmol), benzaldehyde (1 mmol) and aniline (1 mmol). The reactions were carried out at room temperature in the presence of 5 mL of ethanol for 72 h. The obtained compounds were isolated and characterized by ^{1}H NMR. The MgBi catalyst showed high catalytic efficiency, affording a crude yield of 68% and conversions above 99% for 2-(anilino(phenyl)methyl)cyclohexan-1-one, associated with a diastereoselectivity of 82:17 (*anti:syn*). In contrast, catalysts comprising phase mixtures based solely on Mg or Bi showed lower yields of 10% and 37%, respectively, predominantly forming the*anti*-2-(anilino(phenyl)methyl)cyclohexan-1-one isomer, with diastereoselectivities of 99:1 and 94:5 (*anti:syn*). These results highlight MgBi as a promising heterogeneous catalyst that can significantly influence the diastereoselectivity of the Mannich reaction.

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The authors acknowledge Fundação Araucária and CNPq for financial support for this study, PPGQ-UTFPR, and UTFPR.

Di-hidropirimidinonas sintetizadas em meio reacional contendo Tween® 80 em água destilada.

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Palavras Chave:*Di-hidropirimidinonas,Biginelli,surfactantes.*

Highlights

Biginelli synthesis using emulsified media; analysis of the formation and size of Tween® 80 micelles in water; comparison of yields and reaction times with the classical reaction using ethanol.

Resumo/Abstract

Di-hidropirimidinonas (DHPMs) são moléculas heterocíclicas que possuem diversas aplicações na área da saúde e são obtidas a partir da síntese de Biginelli, utilizando solventes orgânicos voláteis (SOVs) como meio reacional. Neste trabalho, busca-se a substituição dos SOVs por Tween® 80 em água, por ele ser um tensoativo não iônico que já é utilizado como emulsificante dentro da indústria química, na tentativa de obter um meio mais verde e potencialmente reutilizável.

Durante o desenvolvimento do projeto, foi realizada a análise por espalhamento de luz dinâmico (DLS), na qual se observou que a concentração micelar do Tween® 80 em água (% m/m) é de 2,5 à 10 %. Também foi avaliada a concentração micelar na presença dos reagentes da reação (acetoacetato de etila, ureia e benzaldeído e FeCl3). Ficou demonstrado que quando se utiliza 5% de Tween® 80 % em água (% m/m) , obtém-se um tamanho de micela de 390,5 nm, demonstrando que ocorre a inserção dos reagentes na estrutura supramolecular que antes apresentava o tamanho de 9,73 nm. Foram realizadas reações variando a concentração das emulsões entre 2,5, 5 e 10 %, com aquecimento, seguindo as condições da reação clássica com etanol (C_2H_5OH) e a temperatura ambiente como foi analisado no DLS, essas com duração de 24h. Os resultados podem ser observados na Tabela 1, sendo utilizados como parâmetros de comparação o tempo reacional e o rendimento. Observa-se que, em relação ao tempo reacional, a concentração ótima de Tween® 80 em água foi de 10% . Contudo, a recuperação das DHPs do meio micelar tem se mostrado desafiadora (rendimentos, Tab. 1). No momento, estamos buscando desenvolver métodos mais eficientes e ambientalmente adequados para a extração dos produtos do meio micelar de Tween® 80 em água .

Reação	Meio	[%]	Tempo (h)	Rendimento (%)
1	EtOH*	--	2	60,49
2	Tween® 80 + H_2O*	2,5	3	34,76
3	Tween® 80 + H_2O*	5	2,5	30,58
4	Tween® 80 + H_2O*	10	2	30,66

* Todas as reações foram realizadas utilizando 5 mL de meio

Tabela 1: Resultados dos tempos reacionais e rendimentos

Distribution of Terpenes and Phenylpropanoids and Antioxidant Potential of Ocimum Essential Oils from Amazonian Markets.

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Palavras Chave:*Lamiaceae, monoterpenes, phenylpropanoids, DPPH.,Lamiaceae, monoterpenes, phenylpropanoids, DPPH.*

Highlights

Chemical diversity among*Ocimum*species commercialized in Amazonian markets. Essential oils were rich in phenylpropanoids and terpenes with significant antioxidant activity.

Resumo/Abstract

The standardization of basil oil (*Ocimum*spp.) products is a key requirement to ensure their quality, efficacy, and safety. Several studies have reported the occurrence of chemical and botanical polymorphism among the species. In this study, ten samples of*Ocimum*species were collected in the free market of Belém (PA) and São Luís (MA) cities, and their essential oils (EO) were extracted by hydrodistillation using the Clevenger apparatus for 3h. The chemical composition of EO of*Ocimum*sp. (3 spp), O. micranthum, O. basilicum, O. americanum (2 spp.) and O. gratissimum (2 spp.) was analyzed by Gas-Chromatography/Mass spectrometer, and the antioxidant activity was performed by DPPH method. The oil yield ranged from 0.7-2.3% and displayed as main compounds (>10%) monoterpenes and phenylpropanoids such as methyl eugenol (0.1-72.8%), E-Methyl cinnamate (0.1-65.4%), Timol (0.11-59.1%), Methyl chavicol (0.03-37.4%), Eugenol (0.1-28.9%) and Linalol (0.1%-17.6%) highlighting a higher chemical variability. Hierarchical cluster analysis with heat mapping of the chemical composition identified six distinct chemical groups: Group I (Ogra1) with high concentrations of monoterpene hydrocarbons (HM, 39.3%) followed by phenylpropanoids (PP, 34.0%); Group II (Ogra2 and Osp1) was rich in PP (53.5-61.6%); Group III (Ocam) was distinguished by having the highest content of oxygenated monoterpenes (OM, 73.4%) followed by sesquiterpene hydrocarbons (SH, 22.0%); Group IV (Osp3) had the highest content of SH (23.13%) despite the predominance of PP (51.36%); Group V (Osp2 and Oame2) was formed by samples rich in PP (59.3-66.0%); Group VI (Omic, Obas and Oame1) was characterized by mean values of PP (30.5-37.7%) and OM (28.6-35.8%). IC50 values between 60.75±12.2 and 376.92±54.02 µg/mL indicate high to moderate antioxidant activity, respectively, reinforcing the importance of characterizing such species.

Agradecimentos/Acknowledgments

CNPq.

EDA complex-mediated synthesis of unsymmetrical selenides under white-light irradiation

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Palavras Chave:*organic selenides,diazonium salts,EDA complex,compact fluorescent lamp,photochemical reaction.*

Highlights

EDA complex-mediated preparation of unsymmetrical selenides using diselenides and diazonium salts in the presence of pyridine under white-light irradiation.

Resumo/Abstract

A photochemical reaction corresponds to a chemical transformation initiated by the absorption of light in the ultraviolet, visible, or infrared regions of the electromagnetic spectrum.[1] EDA complexes, also referred to as charge-transfer complexes, can play an important role in photochemical transformations.[2] In this work, an EDA complex was employed in the preparation of unsymmetrical selenides (**1**) under white-light (CFL) irradiation, avoiding the use of high-energy irradiation[3] and metal- or organic-based photocatalysts.[4] Initially, arenediazonium salts (**2**) were prepared from the corresponding anilines, isoamyl nitrite, and tetrafluoroboric acid in acetic acid.[5] The reaction between diphenyl diselenide (**3**) and 4-methoxybenzenediazonium tetrafluoroborate (**2a**) in the presence of pyridine in acetonitrile under white-light (CFL) irradiation was optimized, affording 4-methoxyphenyl phenyl selenide (**1a**) in 97% yield, as determined by ^{1}H NMR using an internal standard (1,3-dinitrobenzene). The optimized conditions are being applied to the preparation of unsymmetrical selenides (**1**) (**Scheme 1**).

The developed transformation presumably occurs via the formation of an EDA complex between the diazonium salts (**2**) and pyridine,[6] which is photoactivated in the presence of white-light (CFL), leading to the formation of aryl radicals. Experiments to elucidate the mechanism are currently underway.

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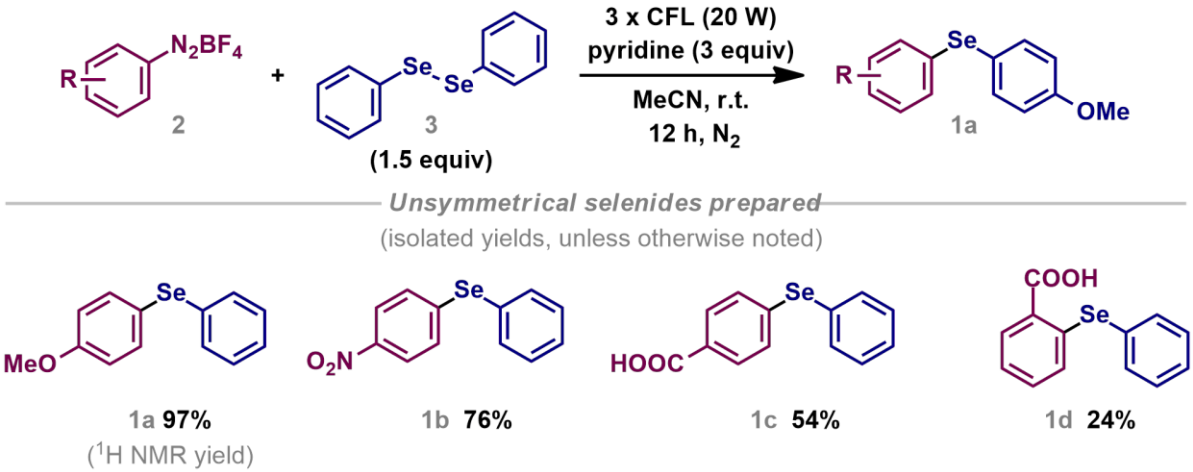
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Scheme 1. White-light-induced synthesis of unsymmetrical selenides (1) via an EDA complex.

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Effect of N-alkyl chain length of imidazolium carbene precursors on the oxidation of aromatic aldehydes in water

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Palavras Chave:*imidazolium,carbene,NHC,oxidation,selectivity*

Highlights

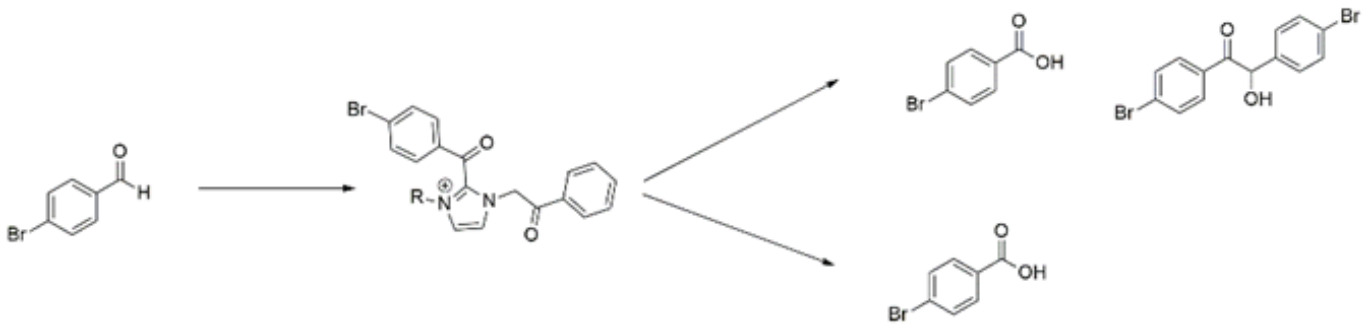
Two imidazolium salts with*N*=methyl and dodecyl form transient carbenes in water; carboxylic acid selectivity depends on*N*-alkyl size.

Resumo/Abstract

Carbenes are important compounds that can be applied as organocatalysts and metal ligands for different reactions (Khatana, Synthesis 2018). An important subclass of this type of compound is the so-called*N*-heterocyclic carbenes (NHCs) derived from imidazolium rings. Due to their high basicity, these NHCs are rarely explored in aqueous media. Therefore, overcoming this challenge can contribute significantly to green chemistry. As recently demonstrated by our group, the introduction of a long alkyl chain on the nitrogen of the imidazolium group favors the formation of transient and active NHC species (Alves, J. of Mol. Liq. 2023). In this context, here we developed Me-AcIm and Dod-AcIm (Me=methyl and Dod=dodecyl), imidazolium salts that can generate NHC species in an aqueous medium.

The catalytic activity of both salts was evaluated in the oxidation of 4-bromobenzaldehyde to the respective carboxylic acid in aqueous medium in the presence of KOH and 10 mol% of the imidazolium salts for 24 hours at 60 °C. The yield and selectivity of the reactions were evaluated by ^{1}H NMR.

For Dod-AcIm, the yield to 4-bromobenzoic acid was approximately 70 %, and no side product was observed. Conversely, for Me-AcIm the yield of 4-bromobenzoic acid was 40 % along with about 44 % yield of the respective benzoin. The control reaction, conducted in the same conditions but without the pre-NHCs, led to a mixture of 10% of carboxylic acid and 10% of 4-bromobenzyl alcohol, confirming that only the Canizzaro reaction took place. Based on these results it is noted that both salts can generate NHC species, with Dod-AcIm showing a higher selectivity toward aldehyde oxidation. Additional studies are being carried out to expand the reaction scope and application.



Caminho reacional da oxidação catalisada do 4-bromobenzaldeido

Agradecimentos/Acknowledgments

CNPq, CAPES, FAPESC, INCTCatálise

Efficient Design of Deep Eutectic Solvents and Evaluation on Carbonyl Condensation Reactions

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Palavras Chave:*Deep Eutectic Solvents, Sustainable synthesis, Thermal Behavior.*

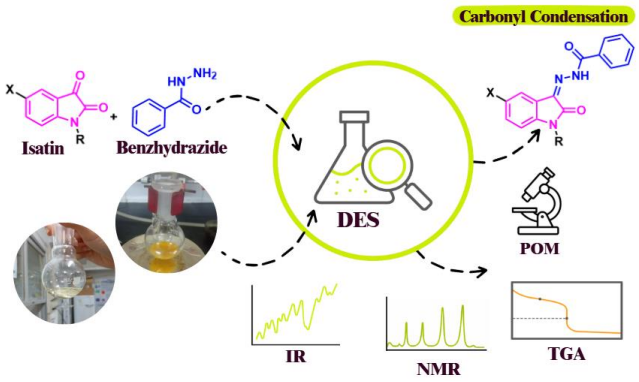
Highlights

Deep eutectic solvents were efficiently synthesized and characterized as stable reaction media. The ChCl:p-TSA system enabled fast N-acylhydrazone synthesis with high yields.

Resumo/Abstract

The search for sustainable alternatives to traditional organic solvents has driven the development of new catalytic systems aligned with the principles of Green Chemistry. In this context, deep eutectic solvents (DES) stand out for their low cost, ease of preparation, biodegradability, and the ability to tune physicochemical properties such as viscosity and density.[1] Therefore, this work aimed to synthesize and characterize DES for their application in the synthesis of N-acylhydrazones derived from*N*-allyl and benzyl isatins. Two different DES were synthesized using choline chloride (ChCl) or benzalkonium chloride (BZK) as hydrogen bond acceptors and p-toluenesulfonic acid (*p*-TSA) as the hydrogen bond donor. The system formation was evaluated using polarized light optical microscopy (POM), and the system was characterized by IR, NMR, DSC, and TGA. POM analysis revealed the influence of the system's molar ratios, enabling identification of suitable proportions for the formation of stable DES. IR, NMR, and DSC characterizations confirmed the DES formation and provided information about their structural interactions and thermal behavior. Both DES were applied in a standard reaction system using isatin and benzhydrazide as substrates, with the aim of evaluating catalytic efficiency and determining optimal reaction conditions. ChCl:*p*-TSA system showed the best performance, standing out with a reaction time of 1 minute and a yield of 95%, while the BZK:*p*-TSA DES resulted in the product in 10 min and 85% of yield. After determining the optimal reaction conditions, a series of halogen-substituted N-acylhydrazone was synthesized in 1 to 120 minutes and 86-95% of yield. Thus, in this work, it was concluded that the DES were synthesized and applied as stable solvents in carbonyl condensation reactions.

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Analysis of deep eutectic solvents and their application in the synthesis of N-acylhydrazones.

Agradecimentos/Acknowledgments

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Efficient One-Pot Flow Synthesis of THC-Type Cannabinoids via Methanesulfonic Acid Catalysis

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Palavras Chave:*THC,continuous flow,synthesis,THC,continuous flow,synthesis*

Highlights

Study of the one-pot synthesis of THC-type cannabinoids (Δ⁹-THC and Δ⁸-THC) using acid catalysis with methanesulfonic acid and its adaptation to continuous-flow processing.

Resumo/Abstract

Cannabis sativa, a plant native to Central Asia, has been used by humans for millennia.[1] Its pharmacological effects are mainly attributed to phytocannabinoids, particularly cannabidiol (CBD) and THC-type cannabinoids such as Δ⁸-THC and Δ⁹-THC.[2] Δ⁹-THC is the primary psychotropic constituent and is commercially available as dronabinol for the treatment of HIV/AIDS-related anorexia and chemotherapy-induced nausea.[3] In contrast, Δ⁸-THC displays milder psychoactive effects and is considered a promising therapeutic alternative for sensitive populations.[4] The literature reports several examples of THC-type cannabinoid synthesis, typically obtained from CBD via intramolecular cyclization.[5,6]

This work explores the one-pot synthesis of THC-type cannabinoids (Δ⁹-THC and Δ⁸-THC). The Friedel–Crafts reaction between menthadienol and olivetol catalyzed by methanesulfonic acid was investigated.[7] The effects of solvent, temperature (0–50 °C), and catalyst concentration (10–50 mol%) were evaluated. Conversion and selectivity were determined by GC-FID, and products were characterized by GC-MS and ^1H/^13C NMR spectroscopy.

CBD was identified as a non-isolated reaction intermediate, and its conversion to THC was mainly influenced by reaction time. High-purity Δ⁸-THC was obtained after 4 h at 50 °C using 50 mol% MsOH, whereas higher selectivity toward Δ⁹-THC was observed after 2 h under the same conditions, supporting the Δ⁹-THC to Δ⁸-THC isomerization pathway. Solvent effects primarily influenced conversion rates. Ongoing studies focus on improving selectivity, particularly toward Δ⁹-THC, and adapting the optimized conditions to continuous-flow systems.

Eletrossíntese Orgânica Aplicada a Reações de Redução e Síntese de Heterociclos

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Palavras Chave:*Organic Electrosynthesis, Reduction reactions, Heterocycles,Organic Electrosynthesis, Reduction reactions, Heterocycles,Organic Electrosynthesis,Heterocycles,Reduction reactions*

Highlights

Organic electrosynthesis enables efficient reduction reactions and heterocycle synthesis under mild, controlled, and more sustainable conditions, offering an alternative to traditional methods.

Resumo/Abstract

Organic electrosynthesis has emerged as a powerful and sustainable approach for promoting redox transformations, offering an alternative to traditional methods that rely on stoichiometric reagents. By using electric current as a clean and tunable reagent, electrosynthetic strategies enable precise control over reaction pathways while minimizing waste generation and improving safety profiles. This presentation will focus on the application of organic electrosynthesis in reduction reactions and in the construction of heterocyclic frameworks. Emphasis will be placed on recent developments demonstrating the efficient generation of reactive intermediates under mild conditions, as well as on the selective formation of C–C and C–heteroatom bonds. In particular, examples involving the electrochemical reduction of functional groups and the synthesis of nitrogen- and oxygen-containing heterocycles will be discussed. Mechanistic aspects will also be addressed, highlighting how electrochemical parameters such as current density, electrode material, and electrolyte composition can influence reactivity and selectivity. The potential of electrosynthesis to access novel reactivity patterns and streamline synthetic routes will be considered, reinforcing its relevance in modern organic synthesis.

Agradecimentos/Acknowledgments

FAPEMIG (APQ-01259-24), CNPq (401402/2025-8), and CAPES (Finance code 001).

Elucidating Crystallization Mechanisms of Cyclodextrin Inclusion Complexes: Insights Into a Novel Structure Composed of β-CD/TTA-H

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Palavras Chave:*Inclusion complexes,Crystallization mechanism,Cyclodextrins,Supramolecular structure*

Highlights

Crystallization mechanisms were proposed for cyclodextrin inclusion complexes using CCDC structures and one newly obtained structure, including a novel β-CD/TTA-H complex.

Resumo/Abstract

Cyclodextrins (CDs) are capable of forming host-guest complexes by intermolecular interactions. This kind of supramolecular structure, known as an inclusion complex, is relevant because it enhances properties of guest molecules, such as water solubility and photostability.[1] In this context, the present study aims to propose crystallization mechanisms and to evaluate similarities between nine crystal structures of CDs inclusion complexes, using a newly determined structure composed of β-CD/TTA-H (hydrated TTA, Fig. 1) as the main reference, contributing to the development of crystal engineering. The TTA molecule forms stable complexes with Eu^{3+} ions that are useful for sensors and bioimaging, representing an interesting molecular model. Encapsulation may help protect these complexes from quenching agents.[2] To fulfill the objectives, supramolecular clusters of each structure were identified, also contact area data (using VDP) and stabilization energies (DFT, ωB97x-D/ccpVDZ basis) between the dimer molecules forming each supramolecular clusters were analyzed.[3] The results indicate that guest molecules may influence the crystal packing through differences in lattice parameters compared to CDs, although some inclusion complexes are isostructural with the macrocycle alone. Intercomponent interactions were determined and quantified by QTAIM and GAI analysis,[4] showing that the most important interactions to stabilize the inclusion complexes were mainly by non-classical hydrogen bonds of the CH•••X type (X=S, O, π carbons) and CH•••HC interactions. The crystallization mechanism of β-CD/TTA-H features a well-defined nucleus that governs the crystal packing, whereas this is less evident for the other studied structures, which present different energetically stable nuclei. 1. D'Agostino, L.*et al.*β-CD Sunscreens.**ACS SCE**(2020); 2. GUO, Y.*et al.***Int. J. Mol. Sci.**23, 6597 (2022); 3. MARTINS, M. A. P.*et al.***RSC Adv.**4, 44337 (2014); 4. KEITH, T. A.*AIMAll*, v14.11.23 (2014).

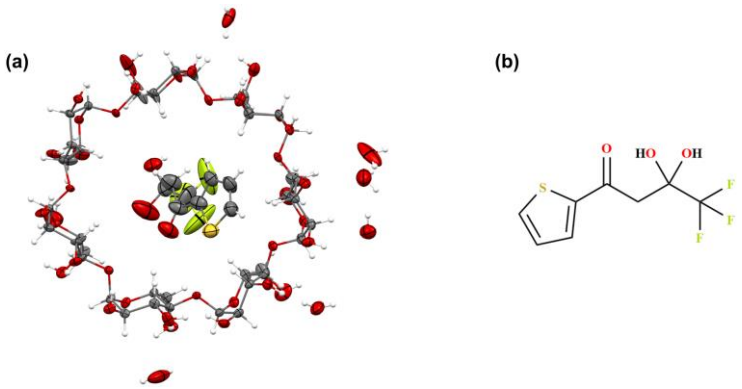


Figure 1. (a) Crystal structure of β-CD/TTA-H, (b) the hydrated 2-thenoyltrifluoroacetone (TTA-H).

Agradecimentos/Acknowledgments

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N-arylation of 4-aminopyrrolo[2,1-f]triazine via Ullmann Reaction

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Palavras Chave:*4-aminopyrrolo[2,1-f]triazine,4-aminopyrrolo[2,1-f]triazine,Ullmann Reaction,N-arylation*

Highlights

The investigation of a protocol to access the*N*-arylation of 4-aminopyrrolo[2,1-*f*]triazine was conducted. The application of Ullman reaction provided the product in 71% yields.

Resumo/Abstract

4-aminopyrrolo[2,1-*f*]triazine is an important heterocycle present in diverse bioactive molecules. It is present in Remdesivir, the first pharmaceutical approved for the treatment of COVID-19, and is the core of drugs like Avapritinib, an antineoplastic agent, and Rogaratinib, an inhibitor of FGFR1-3.[1] Owing to its importance, modifications in this core have gained prominence in recent years. In literature, alkylation protocols are already described using a palladium-catalyzed protocol, however, arylation reactions are still scarce, and there are no optimized methodologies for this heterocycle.[1] To this purpose, the Ullmann Reaction is an alternative, since it permits the arylation of amines using copper as a catalyst and cheap auxiliary ligands like amino acids.[2]

In this work, the arylation of 4-aminopyrrolo[2,1-*f*]triazine was performed applying the Ullmann Reaction. An optimization is being conducted (Table 1), and the reaction solvent, temperature, base, and loading of catalyst and ligand have already been evaluated. In this investigation, dioxane demonstrated better results compared to other solvents, and the temperature evaluation suggested a sensitivity of the reaction to small changes. This study demonstrated that potassium*tert*-butoxide was the best base, and its excess promoted byproducts generation, impacting in reaction yields. Furthermore, the variation of catalyst and ligand loading indicated that small amounts of these reagents proved equally efficient. In the literature, the use of*N,N′*-dibenzyloxalamide has proven promising, however, the low cost of L-proline is a highlight of this protocol. Further studies will be conducted evaluating other modifications to achieve better yields and thus, in the future, construct a scope of molecules.

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Entry	Solvent	Base (equiv.)	Catalyst loading	Ligand loading	Temperature (°C)	Yield (%)
1	DMF	KO^{t}Bu (3.0)	20 mol%	40 mol%	95	22
2	Dioxane	KO^{t}Bu (3.0)	20 mol%	40 mol%	95	42
3	Butanol	KO^{t}Bu (3.0)	20 mol%	40 mol%	95	21
4	Dioxane	KO^{t}Bu (3.0)	-	-	95	0
5	Dioxane	KO^{t}Bu (3.0)	-	40 mol%	95	0
6	Dioxane	KO^{t}Bu (3.0)	20 mol%	-	95	26
7	Dioxane	KO^{t}Bu (3.0)	20 mol%	40 mol%	105	67
8	Dioxane	KO^{t}Bu (3.0)	20 mol%	40 mol%	115	59
9	Dioxane	KO^{t}Bu (3.0)	20 mol%	40 mol%	120	59
10	Dioxane	Et_3N (3.0)	20 mol%	40 mol%	105	0
11	Dioxane	Na_2CO_3 (3.0)	20 mol%	40 mol%	105	0
12	Dioxane	NaO^{t}Bu (3.0)	20 mol%	40 mol%	105	29
13	Dioxane	KO^{t}Bu (2.0)	20 mol%	40 mol%	105	24
14	Dioxane	KO^{t}Bu (4.0)	20 mol%	40 mol%	105	71
15	Dioxane	KO^{t}Bu (4.5)	20 mol%	40 mol%	105	72
16	Dioxane	KO^{t}Bu (4.0)	10 mol%	20 mol%	105	71

Table 1. Reaction optimization.

Agradecimentos/Acknowledgments

The authors are grateful for the generous financial support from CAPES, CNPq, UFJF, FAPEMIG and Microbiologica Química e Farmacêutica Ltda.

N-Functionalization of 4-aminopyrrolo[2,1-f][1,2,4]triazine via Iron-Catalyzed Borrowing Hydrogen.

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Palavras Chave:*4-aminopyrrolo[2,1-f][1,2,4]triazine,Green chemistry*

Highlights

An optimized protocol for the functionalization of 4-aminopyrrolo[2,1-*f*][1,2,4]triazine via Iron-catalyzed Borrowing Hydrogen methodology as a more economical and sustainable alternative.

Resumo/Abstract

Amines and their derivatives are indispensable building blocks in the pharmaceutical, fine chemical, and natural product industries, holding high relevance for chemical research. Although classical methodologies for C–N bond formation, such as hydroamination and Buchwald–Hartwig coupling, are well-established, they can generate unwanted waste and byproducts.[1,2]

A greener strategy for achieving N-alkylated molecules would be through the Hydrogen Borrowing (HB) methodology, utilizing an iron-based metallic catalyst. In this approach, alcohols serve as alkylating agents; they are oxidized via the hydrogen transfer method to their carbonyl intermediates, followed by in situ condensation with an amine to generate an imine. This imine is then hydrogenated to produce the N-alkylated product, with water as the sole byproduct. [1,3]

A nucleophile of interest is pyrrolo[2,1-*f*][1,2,4]triazin-4-amine, an*N*-fused heterocycle recognized for its significant biological profile. It is present in several antiviral agents, such as Remdesivir, an FDA-approved drug during the COVID-19 pandemic.[4] The functionalization of such molecules through sustainable methods is of great importance for the improvement and creation of potential drugs.

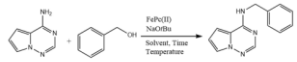
The optimized protocol employed an Fe(II) complex as a catalyst and NaOtBu as a base. Using benzyl alcohol as the alkylating agent, the reaction was conducted in a sealed tube at 140 °C for 72 h in the presence of molecular sieves. This approach provided the product with an isolated yield of 63% after purification.

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(2) BAINS, Amreen K.*et al*.*ACS Catalysis*, v. 9, n. 10, p. 9051–9059,**2019.**

(3) BALA, Manju*et al*.*Green Chemistry: Green Chemistry Resource*: GC, v. 15, n. 6, p. 1687–1693,**2013.**

(4) DURÃES PEREIRA, Vinícius Rodrigues*et al.European Journal of Organic Chemistry*, v. 28, n. 42,**2025.**



Entry	Solvent	Time (h)	Temp. (°C)	Catalyst (mol%)	Benzyl Alcohol (Equiv.)	Base (Equiv.)	Yield (%)
1	Toluene	12h	100	1 mol%	1	2	nd
2	DMSO	24	140	1.5 mol%	1.5	2.5	3.4
3	Dioxane	24	140	1.5 mol%	1.5	2.5	11.5
4	Dioxane	48	140	1.5 mol%	1.5	2.5	14.4
5	Dioxane	48	140	3 mol%	1.5	2.5	12.6
6	Dioxane	60h	140	1.5 mol%	1.5	2.5	33
7	Dioxane	72h	140	1.5 mol%	1.5	2.5	39.6
8	Dioxane	96h	140	1.5 mol%	1.5	2.5	30
9	Dioxane	72h	140	1.5 mol%	1.5	1	6.3
10	Dioxane	72h	140	1.5 mol%	1.5	8	nd
11*	Dioxane	72h	140	1.5 mol%	1.5	2.5	19.7
12	Dioxane	72h	140	1.5 mol%	2	2.5	26
13	Dioxane (30 eq)	72h	140	2 mol%	2	3	58.3
14	Dioxane (30 eq)	72h	140	3 mol%	3	4	46.1
15	Dioxane (20 eq)	20h	100	2 mol%	2	3	36.1
16	Dioxane (20 eq)	48	100	2 mol%	2	3	29.9
17**	Dioxane (30 eq)	72h	140	2 mol%	2	3	63.4

* Using K'OBu as a base.

** Under 3Å molecular sieves.

Optimization of reaction conditions.

Agradecimentos/Acknowledgments

The authors are grateful for the generous financial support from CAPES, CNPq, UFJF, FAPEMIG, and Microbiológica Química e Farmacêutica LTDA

Estratégias Sintéticas para a Funcionalização de Cumarinas como Blocos de Construção Versáteis e Multifuncionais

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Palavras Chave:*Heterociclos;,versatilidade sintética;,sistemas bioativos;,propriedade fotofísicas;,materiais funcionais;*

Highlights

Cumarinas atuam como blocos de construção versáteis; a funcionalização racional constitui uma estratégia robusta para o desenvolvimento de moléculas com propriedades ajustáveis e aplicações variadas.

Resumo/Abstract

As cumarinas constituem uma classe de compostos heterocíclicos amplamente reconhecida por sua versatilidade estrutural e relevância em diferentes áreas da química, incluindo química medicinal, ciência dos materiais e sistemas fotofuncionais. Nesse contexto, esta palestra abordará estratégias sintéticas para a funcionalização de cumarinas, destacando sua utilização como blocos de construção versáteis e multifuncionais. Serão apresentados métodos eficientes e seletivos para a modificação estrutural em diferentes posições do arcabouço cumarínico. Serão ainda mostradas funcionalizações pontuais, bem como estratégias de conjugação com diferentes sistemas, visando a modulação de propriedades eletrônicas, fotofísicas e biológicas. Além disso, serão abordadas metodologias que possibilitam a construção de arquiteturas moleculares mais complexas a partir de esqueletos cumarínicos, ampliando seu potencial como plataformas sintéticas. Por fim, serão apresentados exemplos representativos desenvolvidos no Laboratório de Síntese Orgânica Aplicada (LabSOA), do Instituto de Química da Universidade Federal Fluminense, evidenciando aplicações desses compostos em contextos que incluem bioatividades e materiais funcionais, tais como células solares, sondas fluorescentes e sensores ópticos. Os resultados demonstram que a funcionalização racional de cumarinas constitui uma estratégia robusta para o desenvolvimento de moléculas com propriedades ajustáveis e aplicações multidisciplinares.

Agradecimentos/Acknowledgments

Capes, CNPq e Faperj

Expandindo o espaço químico de reações multicomponentes catalisadas por enzimas sintéticas

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Palavras Chave:*: reações multicomponentes, Synzyme, química verde,reações multicomponentes,Synzyme,química verde,PEI*

Highlights

Enzimas sintéticas de Polietilenoimina (PEI) como catalisadores eficientes em reações multicomponentes, alinhado aos princípios da química verde.

Resumo/Abstract

A polietilenimina (PEI) é um polímero altamente funcionalizado, capaz de atuar como um sistema catalítico multifuncional, promovendo ativação ácido–base, estabilização de intermediários e organização supramolecular dos reagentes. Essas características permitem que o material mimetize parcialmente o microambiente catalítico de enzimas, justificando sua classificação como*synzyme*.
A combinação de PEI com líquidos iônicos (PEI·LI) potencializa essas propriedades, originando sistemas catalíticos mais eficientes e sustentáveis, capazes de operar sob condições brandas e, frequentemente, livres de solvente. Nesse contexto, os synzymes de PEI emergem como alternativas promissoras dentro da química verde, aliando eficiência catalítica, versatilidade estrutural e baixo impacto ambiental.
Diversas reações multicomponentes (RMC) foram desenvolvidas utilizando sistemas PEI·LI, apresentando bons rendimentos e conduzidas sob condições ambientalmente adequadas.

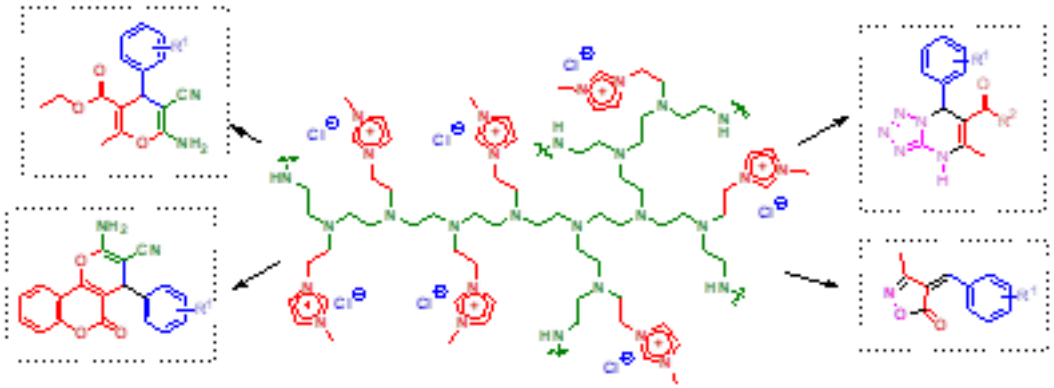


Figura 1. Estrutura do catalisador de PEI à base de imidazólio (enzima sintética) usado em RMC

Agradecimentos/Acknowledgments

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Experimental and Computational NMR Study of a New Polyketide Isolated from Talaromyces pinophilus

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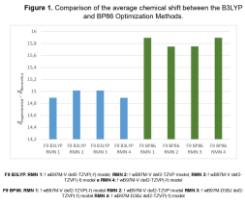
Palavras Chave:*Talaromyces pinophilus,NMR,theoretical chemical shifts,(−)-R-talaropinophiloic acid*

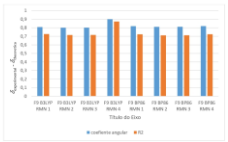
Highlights

A new polyketide was isolated from a fungus and elucidated by NMR with computational support. DFT matched experiment; carbonyl 13C shifts are sensitive, requiring explicit solvent and aggregation Now.

Resumo/Abstract

The new polyketide (-)-R-talaropinophiloic acid was isolated from Talaromyces pinophilus J6 found on Euphorbia umbellata leaves. Its structure was determined by NMR and validated computationally. Their chemical structures were elucidated by Nuclear Magnetic Resonance (NMR), and computational NMR calculations were carried out to support the proposed structures.
After a conformational search and geometry optimization at the B3LYP-D3 and BP86 levels, shielding calculations were tested with various DFT models. The wB97M-D3BJ/def2-TZVP(-f) model, using B3LYP-optimized geometries, provided the best correlation with experimental data (R^2 = 0.87), significantly outperforming the other models (R^2 = 0.71-0.72) and showing reduced systematic error. The results indicate that the exclusion of f-polarization functions plays a more critical role than dispersion corrections for accurate prediction of NMR chemical shifts in methanol solution. However, using BP86-D3 optimized geometries eliminated this advantage, reducing all models to similar, lower accuracy (R^2 ~0.71–0.72). The strong dependence of the calculated ^{13}C chemical shifts on the optimization level is consistent with previous observations that hydrogen bonding induces significant deshielding effects, particularly for carbonyl and adjacent methyl carbons. In hydrogen-bonded systems, an accurate description of the hydrogen-bond geometry is essential, and use of hybrid DFT methods is essential for an adequate description While the core structure was successfully defined, the carbonyl carbon resonances require further investigation, as their chemical shifts appear to be strongly influenced by intermolecular interactions and solvent effects. Ongoing and future studies will therefore focus on explicit solvent calculations and on the modeling of molecular aggregates involving two or more molecules of the compound, aiming to achieve a more accurate description of the carbonyl environments.





Agradecimentos/Acknowledgments

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Formal Synthesis of API Cetirizine

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Palavras Chave:*Levocetirizine,Petasis-Borono-Mannich,Multicomponent*

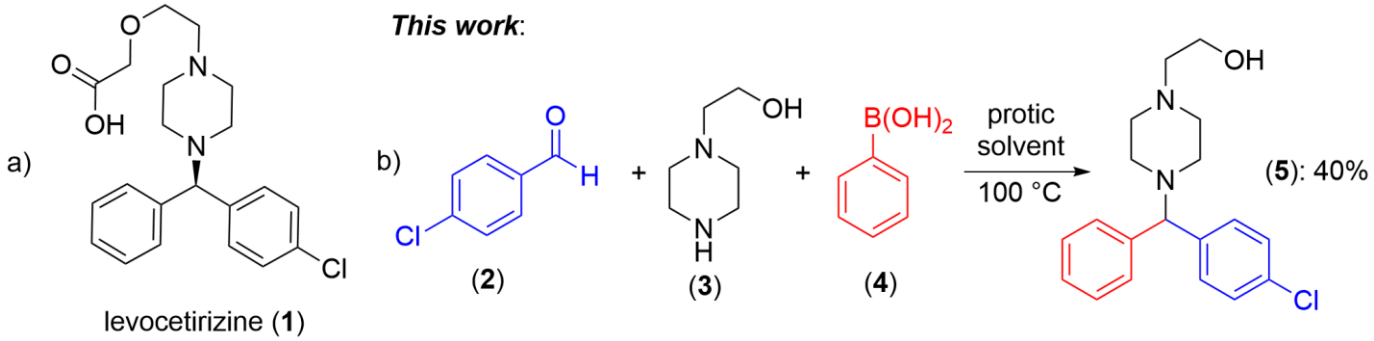
Highlights

An alternative protocol for the synthesis of the cetirizine intermediate was developed based on the Petasis-Borono-Mannich reaction.

Resumo/Abstract

Multicomponent reactions have gained significant prominence in synthetic chemistry due to the advantages they offer over conventional routes, such as the reduction in the number of steps, reaction time, and the need for intermediate purification processes. In this context, the synthesis of active pharmaceutical ingredients (APIs) often involves three or more steps, resulting in limited overall yields. Accordingly, the Petasis–Borono–Mannich (PBM) reaction represents an efficient multicomponent strategy based on the addition of organoboronic acids to imines or iminium ions generated*in situ*through the condensation of amines and aldehydes, with the activation of the boronic acid by a Lewis base being essential for C–C bond formation.

Levocetirizine (1) is an API widely used in the treatment of allergic disorders, exhibiting a favorable pharmacokinetic profile, including high absorption, low sedative effects, and long duration of action. In this work, an alternative synthetic route was developed for the preparation of the cetirizine intermediate 2-(4-((4-chlorophenyl)(phenyl)methyl)piperazin-1-yl)ethan-1-ol, employing commercially available reagents and the Petasis reaction as the key step (Scheme 1). As preliminary results, aldehyde 2, piperazine derivative 3, and boronic acid 4 were reacted in the presence of protic solvent, aprotic solvent, and under solvent-free conditions. To date, under protic solvent conditions and at temperatures above 100 °C, intermediate 5, corresponding to the formal synthesis of the API, was obtained in a single step with a yield of 40% (Scheme 1).



Scheme 1: a) levocetirizine; b) PBM reaction for the preparation of 5.

Agradecimentos/Acknowledgments

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From Coffee Grounds to Tricalysiolides: Cafestol as a Renewable Synthetic Platform

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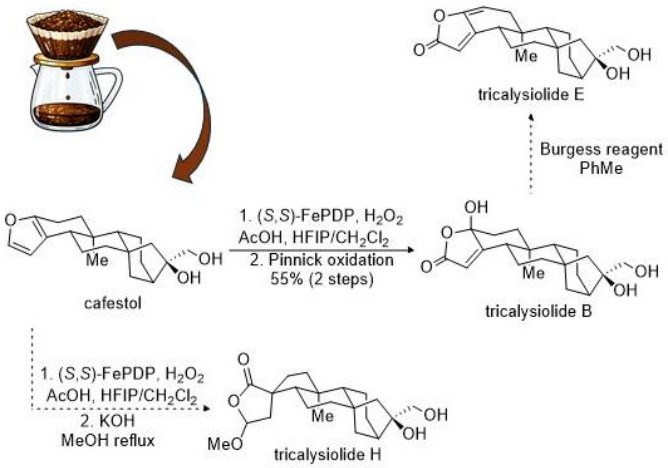
Palavras Chave:*natural products, catalysis, oxidations, metals, C—H bonds*

Highlights

Cafestol is extracted from coffee grounds as a renewable diterpene, serving as a scaffold that enables the synthesis of tricalysiolides.

Resumo/Abstract

Coffee grounds are a renewable source of cafestol, an*ent*-kaurane diterpene structure with a highly complex, rigid scaffold and multiple stereogenic centers that challenged selective chemical transformations. Cafestol stands out as a model substrate for studies that allow the exploration of late-stage oxidation without extensive protecting group manipulations. In this context, tricalysiolides have attracted attention due to their reported biological activities, motivating synthetic efforts toward their synthesis. Herein, we describe the isolation and purification of cafestol from coffee grounds and its use as a precursor for the synthesis of Tricalysiolide B. In addition, we investigate cafestol as a scaffold for a divergent strategy aimed at accessing other tricalysiolides. The proposed approach relies on key steps of oxidation, epoxidation and carbon-skeleton rearrangement. These results highlight the potential of cafestol as a versatile platform to the synthesis of complex molecules.



Reactions from cafestol

Agradecimentos/Acknowledgments

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Green mechanochemical ring opening of epoxides catalyzed by Amberlyst-15 dry

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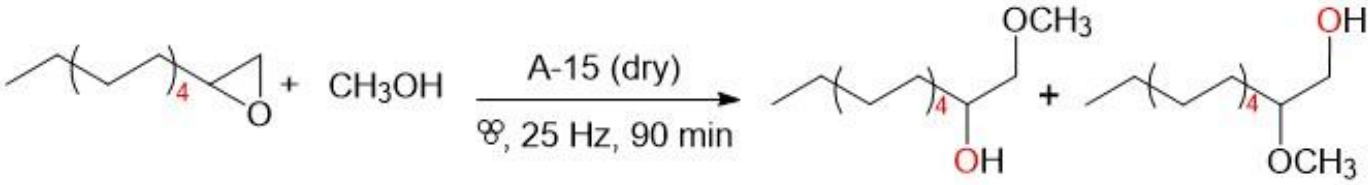
Palavras Chave:*Epoxide,mechanochemistry,heterogeneous catalysis,amberlyst-15,green chemistry*

Highlights

Epoxide ring opening was achieved under mechanochemical conditions using a heterogeneous acid catalyst.

Resumo/Abstract

The ring opening of epoxides is a transformation of great relevance in organic synthesis, enabling the formation of functionalized β-alcohols that are widely used as chemical intermediates [1]. In this work, the ring opening of cyclohexene oxide and 1,2-epoxydecane was investigated using short-chain alcohols (methanol, ethanol, and butanol) as nucleophiles, with dry Amberlyst-15 employed as a heterogeneous catalyst. The reactions were carried out under mechanochemical conditions using an IKA Ultra Turrax device, which stands out for being portable, low-cost, and aligned with the principles of green chemistry, as it enables reduced solvent use and contributes to waste minimization. The results obtained from gas chromatography (GC) analyses demonstrated the efficiency of the proposed catalytic system, particularly for reactions involving cyclohexene oxide. Conversions of 94%, 50%, and 88% were achieved when methanol, ethanol, and butanol were used as nucleophiles, respectively, under mechanochemical conditions. These results indicate the influence of the nature of the alcohol on the efficiency of epoxide ring opening. In parallel, reactions performed with 1,2-epoxydecane showed a strong dependence of conversion on the alcohol employed, with conversions of 91% and 35% observed for methanol and ethanol, respectively, while no reaction was observed with butanol. In addition, GC analyses indicated a mixture of possible isomers in the ring opening of 1,2-epoxydecane, suggesting that Amberlyst-15 does not exhibit selectivity in the opening of this epoxide. As a perspective, ring-opening experiments of 1,2-epoxybutane with different alcohols are currently underway, aiming to expand the scope of the study and to deepen the understanding of the reaction behavior of the system. Furthermore, additional analytical techniques will be employed for the complete structural elucidation of the obtained products.
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Scheme 1 – Mechanochemical Ring Opening of 1,2-epoxydecane with Methanol

Agradecimentos/Acknowledgments

FACEPE, CNPq, Capes, UFPE, CA-DQF.

Heating-based optimization in the synthesis of cannabigerol and its derivatives

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Palavras Chave:*phytocannabinoid, cannabigerol derivatives, bioactive substances, microwave heating, organic synthesis,phytocannabinoid,cannabigerol derivatives,bioactive substances,microwave heating,organic synthesis*

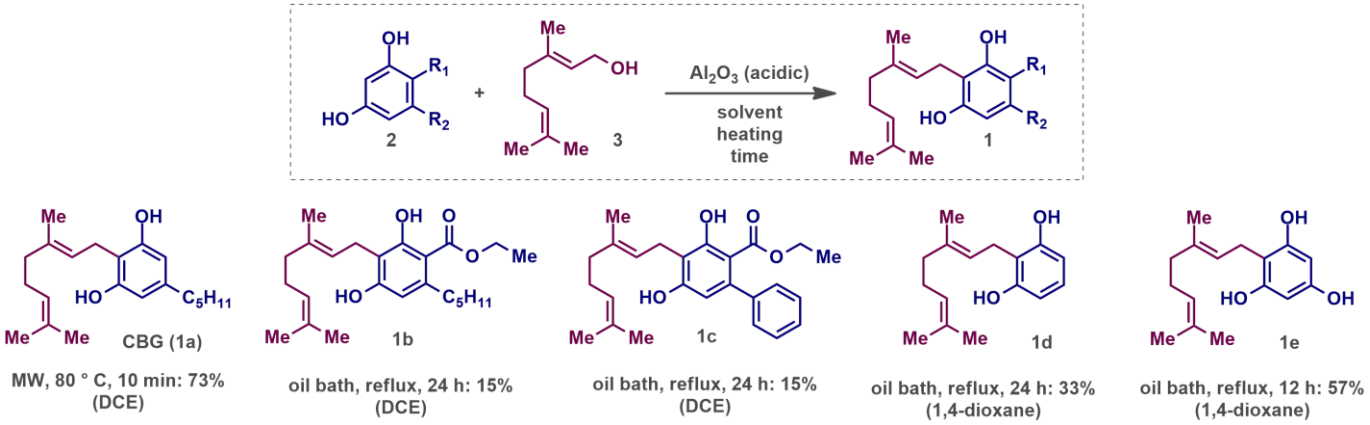
Highlights

Preparation of cannabigerol, a non-psychotropic phytocannabinoid, and its derivatives was optimized using oil bath (6-24 h) and microwave heating (10-180 min).

Resumo/Abstract

Cannabigerol (CBG,**1a**) is a non-psychotropic phytocannabinoid and a biosynthetic precursor of several other classes of phytocannabinoids.[1] It has demonstrated therapeutic potential through interactions with the endocannabinoid system and shows distinct affinities for additional receptor systems, opening promising avenues for medical applications, including anti-inflammatory effects, neuroprotection, glaucoma treatment, and potential anticancer activity.[2] Despite its significance, synthetic approaches to CBG (**1a**) remain limited.[2] In this context, we report the optimization of the preparation of CBG and its derivatives (**1**) via acidic alumina-catalyzed alkylation of resorcinol cores (**2**) with geraniol (**3**), using both oil bath (6-24 h) and microwave heating (10-180 min) (**Scheme 1**). CBG and its derivatives (**1**) were obtained in yields ranging from 15% to 73% (**Scheme 1**). The alkylation reaction was sensitive to substituent group effects, and careful optimization of the reaction conditions was required to minimize multiple alkylations. Studies aimed at further expanding the reaction scope are currently in progress.

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2 Ortuño, J. F.; Ghisolfi, A.; Almansa, R.; Barros, O. S . R.; Sirvent, A.; Sansano, J. M.; Foubelo, F.*Organics***2025**,*6*, 31.
3 Jentsch, N. G.; Zhang, X.; Magolan, J.*J. Nat. Prod.***2020**,*83*, 2587.



Scheme 1. Preparation of CBG and its derivatives (1).

Agradecimentos/Acknowledgments

We are grateful to FAPESP and CNPq for the financial support. K.R. thanks CAPES for the scholarship.

Indaiá palm (Attalea dubia) coconut oil as an alternative feedstock for biodiesel production

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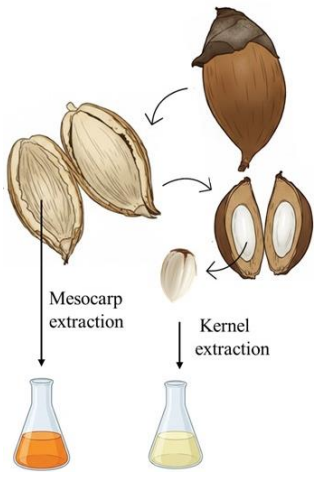
Palavras Chave:*Indaiá palm; renewable feedstock; vegetable oil; characterization; biodiesel*

Highlights

Use of a native plant resource as a renewable energy alternative.
Extraction and characterization of oils from different fruit fractions.
Potential application in biodiesel production.

Resumo/Abstract

The Indaiá palm (*Attalea dubia*) is a species native to Brazil, mainly founded in the Southeast, South, and Central-West regions, and endemic to the Atlantic Forest biome. As a renewable and still little-explored resource for energy purposes, fruits (coconuts) of the Indaiá palm were collected in Domingos Martins, ES, Brazil. After, the fruits were processed, and the kernel and mesocarp were separated. The kernels were crushed, oven-dried at 60 °C for 24 h, and subsequently subjected to hexane extraction for three days. The extract was then filtered, and the solvent was removed using a rotary evaporator. The mesocarp was subjected to a similar procedure. The yields obtained were approximately 46% for the kernel oil and 31% for the mesocarp oil. After extraction, the physicochemical properties of the oils were evaluated. The kernel oil showed higher saponification and lower peroxide values (250.10 mg KOH/g and 0.398 meq/1000 g, respectively) compared to the mesocarp oil, which presented a saponification value of 196.58 mg KOH/g and a peroxide value of 18.297 meq/1000 g. In addition, the acid value, viscosity, moisture content, and density were also determined. Infrared (IR) and proton nuclear magnetic resonance (^{1}H NMR) spectra confirmed the lipid nature of the oils, indicating the presence of ester groups, characterized by the C=O stretching band at ~1743 cm^{-1}, long aliphatic chains (~2923 and ~2854 cm^{-1}), and unsaturation, as well as characteristic triacylglycerol signals in the ^{1}H NMR spectra, with resonances at ~4.0–4.4 ppm and ~5.2–5.3 ppm. The fatty acid profile was determined by gas chromatography to identify the main components. Based on these results, both oils have great potential for energy and biotechnological applications.



Schematic representation of the fruit showing mesocarp and kernel fractions and their oils

Agradecimentos/Acknowledgments

Financial support from FAPES and CNPq and technical and infrastructure support from UFES and LabPetro are acknowledged

Influence of deep eutectic solvent based on choline chloride and glucose as plasticizer for starch films: a study of the physical-chemical properties

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Palavras Chave:*Deep Eutectic Solvent,Starch Film,Choline chloride based*

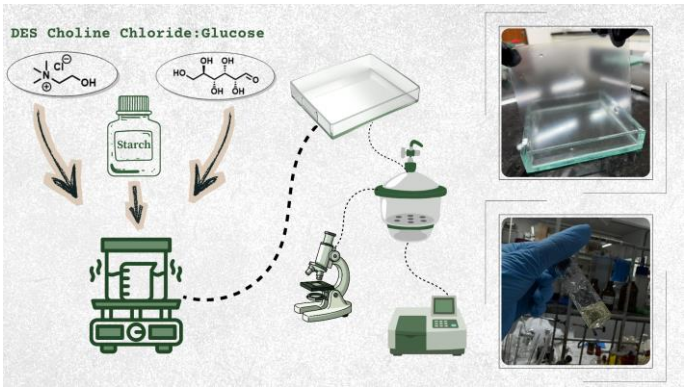
Highlights

The ChCl:Glu Deep Eutectic Solvent (DES) demonstrated strong potential as a sustainable alternative for Starch Film plasticization. New Starch-based Films were successfully obtained using ChCl:Glu.

Resumo/Abstract

Polymers, such as poly(vinyl chloride), polypropylene, and polystyrene, are widely used in packaging due to their durability and strength. However, they exhibit high resistance to degradation, resulting in significant environmental risks. Therefore, recent studies have reported the use of Deep Eutectic Solvents (DES) as a sustainable alternative for developing starch films, owing to their high thermal stability, atomic economy, and low cost.[1] This research focuses on studying the influence of choline chloride and glucose (1:1) on the physical-chemical properties of new starch films in different proportions. Initially, the DES were synthesized in an oil bath at 80°C for 2 h in an equivalent molar ratio. The solvent was characterized by ATR-FTIR and NMR spectroscopy. Afterwards, four films were prepared from a film-forming solution (FFS) by mixing starch with 5% w/v water and placing it in a water bath at 80°C for 30 minutes, with stirring every 5 minutes. Subsequently, glycerol (Gly) and the DES were added as plasticizers, enabling comparison between conventional and alternative plasticizers. The filmogenic solution remained in the water bath for an additional 15 minutes. The gel was then poured onto glass plates and conditioned at ~51% relative humidity at 18°C for 72 h. The gelatinization of the FFS was formed when the temperature reached ~55°C, which is a positive result since the normal temperature for gelatinization is ~80°C. The resulting starch films: Gly 2%; DES 2%; Gly:DES 1:1%; DES 1% were then carefully removed from the casting molds. The thermoplastic films were characterized by thickness, transparency, ATR-FTIR Spectroscopy, Polarized Optical Microscopy (POM), UV–Vis Spectroscopy, and Scanning Electron Microscopy (SEM). In summary, DES was an efficient plasticizer, exhibiting a lower gelatinization temperature and high transparency, with potential for use in food packaging.

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Starch based film preparation and characterization

Agradecimentos/Acknowledgments

The authors are grateful to Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPQ, Coordenação de Aperfeiçoamento Pessoal de Nível Superior – CAPES, and Federal University of Paraíba - UFPB for financial support.

Integração da Síntese Orgânica com Metodologias de Drug Design (in silico) na Busca de Novos Fármacos contra a C. Albicans

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Palavras Chave:*Candida Albicans , Hsp90, Structure Based e Ligand Based Drug Design, Ácido Kójico*

Highlights

Through use of Structure Based and ligand Based Drug Design, the objective of this work is to synthetise new kojic acid derivatives capable of inhibiting the activity of Hsp90 protein.

Resumo/Abstract

A infecção sistêmica por Candida albicans causa mortalidade de 30% a 60% dos pacientes[1]. No Brasil, a taxa de incidência de candidemia é de 2,49 casos a cada 1000 admissões hospitalares, cerca de 2 a 15 vezes maior que nos Estados Unidos e em países europeus[2]. Assim, o desenvolvimento de novos fármacos para contornar os mecanismos de resistência faz-se necessário. As técnicas de Structure Based e Ligand Based Drug Design (SBDD e LBDD), molecular docking e planejamento sintético foram empregadas para o estudo de moléculas com potencial inibitório da enzima Hsp90 (Heat Shock Protein), presente na C. albicans. Foram detalhados os dados cristalográficos e as interações relevantes no sítio drogavel. O radicicol (RAD) foi escolhido como ligante de referência por apresentar boa atividade antifúngica. Contudo, a falta de seletividade para células fúngicas o torna um composto tóxico para uso em humanos3. Considerando sua estrutura molecular, investigou-se moléculas com semelhança estrutural e padrões de orientação espacial capazes de interagir com os mesmos resíduos de aminoácidos que o RAD. Empregando a técnica de molecular docking, selecionaram-se derivados do ácido kójico, pois o anel γ-pirona apresenta boa sobreposição ao anel aromático do RAD e seus substituintes exibiram um padrão de orientação semelhante ao do ligante de referência no sítio drogavel da Hsp90. Além disso, as energias de interação foram analisadas e os derivados AK0001 (-5,1 kJ/mol) e AK0002 (-5,7 kJ/mol), apresentaram resultados promissores nos requisitos estudados (Figuras 1, 2 e 3).

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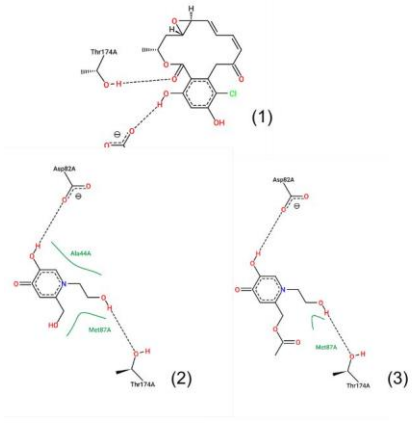


Figura 1 - Mapa de interações em 2D de Hsp90 com (1) Radicicol, (2) AK0001 (3) AK0002.

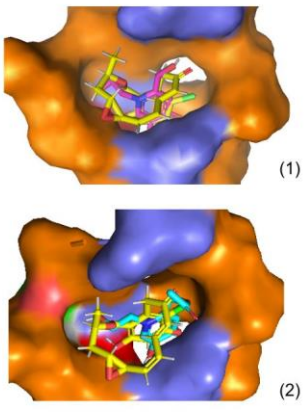


Figura 2 - Mapeamento de direcionamento do Racidicol em relação aos compostos (1) AK0001 (2) AK0002 no sítio drogável da Hsp90.

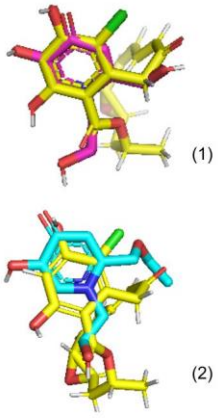


Figura 3 - Sobreposição de (1) AK0001 e (2) AK0002 com o Radicicol.

Interações dos compostos com Hsp90 e sobreposição estrutural de AK0001 e AK0002 com Radicicol.

Agradecimentos/Acknowledgments

Agradeço a Universidade Federal do ABC, CAPES, CNPQ.

Iron-Catalyzed LMCT Photocatalytic Oxidation of Indoles under Visible Light

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Palavras Chave:*Iron catalysis,Ligand-to-metal charge transfer (LMCT),Visible-light-mediated reactions.,Indole oxidation*

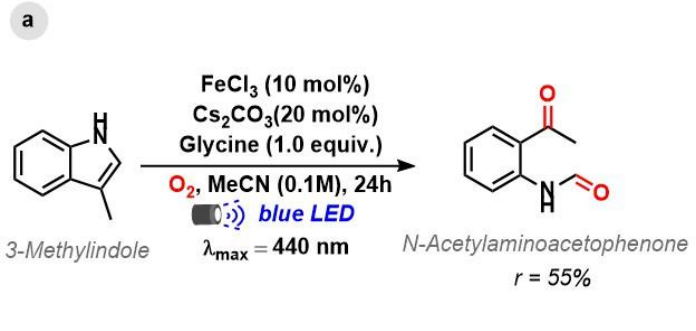
Highlights

An iron-based LMCT photocatalytic strategy enables the Witkop oxidation of indoles under visible light.

Resumo/Abstract

N-Acetylaminoacetophenone derivatives are relevant intermediates in organic synthesis and drug discovery and are commonly obtained through the Witkop oxidation[1] of indole derivatives.[2] Despite their high commercial value, classical methods for this transformation generally rely on hazardous reagents, such as chromic acid, peracids, hypervalent iodine compounds, ozone, or toxic transition metals.[3] Recent advances in visible-light photochemistry, including porphyrin-based photoredox oxidation of indoles[4] illustrate the potential of light-driven strategies to enable milder oxidative processes. In this context, strategies based on ligand-to-metal charge transfer (LMCT) enable the*in situ*generation of reactive species from earth-abundant metal catalysts, such as iron, and have emerged as promising alternatives. In this work, an LMCT-based photocatalytic methodology for the Witkop oxidation is reported, employing iron as the catalyst under visible-light irradiation for the synthesis of*N*-acetylaminoacetophenone derivatives. Several reaction conditions were evaluated (Figure a). Under the optimized preliminary conditions, using 3-methylindole (0.1 mmol) and glycine (0.1 mmol), in the presence of $FeCl_3$ (10 mol%) and Cs_2CO_3 (20 mol%) in acetonitrile under blue-light irradiation (λ= 440 nm), the*N*-acetylaminoacetophenone derivative was obtained in 55% yield (Figure b). These initial results demonstrate the feasibility of the proposed approach, enabling access to*N*-acetylaminoacetophenone derivatives in good yields. Further studies on reaction optimization, substrate scope, and mechanistic investigations are currently underway.

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b

Entry	Conditions	Yield %
1	bubbling O_2 into the solution	55
2	absence Cs_2CO_3	nd
3	absence glycine	5
4	deoxygenated solvent	nd
5	absence of light	nd
6	oxygen atmosphere	30
7	absence $FeCl_3$	nd

a) General reaction. b) Optimization of reaction conditions.

Agradecimentos/Acknowledgments

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Isatin-based N-acylhydrazone as molecular gels: Influence of alkyl chain length and branching on Self-Assembly dynamics

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Palavras Chave:*Molecular gels; N-acylhydrazones; branched alkyl chains.*

Highlights

N-acylhydrazones derived from*N*-alkyl isatins exhibited gelation properties in a variety of solvents, forming colored gels. Branched and short alkyl better stabilize supramolecular self-organization.

Resumo/Abstract

Low molecular weight organogelators (LMWOGs) are formed from self-organization through non-covalent interactions. Self-assembled fibrillar networks (SAFiNs) can immobilize liquid components, exhibiting a dynamic nature with the ability to respond to different stimuli [1]. The*N*-acylhydrazone core intrinsically provides directional hydrogen-bonding capability and, through rational molecular design, can be combined with lipophilic segments, conjugated rings, and spacer groups to generate functionalized architectures suitable for molecular gel formation. Furthermore, the combination of*N*-acylhydrazone and isatin skeletons is noteworthy, as the strong absorption nature of isatin derivatives leads to colored gels [2]. In this context, ten*N*'-(2-oxoindolin-3-ylidene)benzohydrazides were synthesized from*N*-alkylated isatins (*N*-prenyl,*N*-2-ethylhexyl,*N*-hexyl,*N*-dodecyl and*N*-hexadecane) and 2-substituted benzohydrazides (2-H and F). Their gelation properties were also investigated. The synthesis of N-acylhydrazones was carried out using the conventional method, in a medium of ethanol and catalytic acetic acid, with reaction times ranging from 2-7 h and good yields (70-94%). The chemical structures were characterized by ^{1}H and ^{13}C NMR, IR and HRMS. Six compounds formed stable yellow gels in ethylene glycol, propylene glycol, and mineral oil with a minimum gelation concentration (MGC) ranging from 1.3 to 4% w/w. We found that the gelation ability improves for relatively shorter alkyl chains, particularly when branching is present. The isatin-based N-acylhydrazone bearing a branched and relatively shorter alkyl chain*N*-(1-(2-ethylhexyl) formed a transparent gel in mineral oil (Figure). Some compounds formed gels in cyclohexanol,*tert*-butanol, acetonitrile, cyclohexane, and diesel. The gels were examined using SEM and POM.



Chemical structures of all compounds and a photo of the gel 4b

Agradecimentos/Acknowledgments

FAPESQ-PB, UFPB, CAPES and CNPq for scholarships.

Isatin-based semicarbazones as simple and versatile scaffolds for molecular gels

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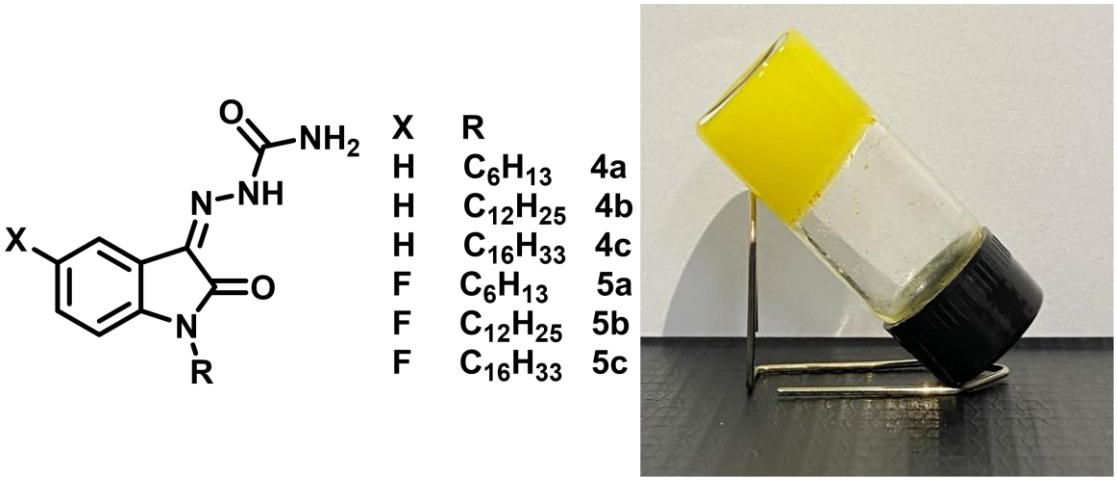
Palavras Chave:*Molecular gels; Semicarbazone; Isatin.*

Highlights

Isatin-derived semicarbazones form efficient molecular gels with MGC values as low as 0.4% (w/w). Gelation behavior is strongly governed by alkyl chain length and the halogen at isatin core.

Resumo/Abstract

Low molecular weight organogelators (LMWOGs), organic semiconductors and other molecular compounds that form self-assembled structures have been gaining significant attention from researchers in recent times [1]. Molecular gels are notable for their ability to hierarchically aggregate into complex supramolecular structures capable of impeding solvent flow. The self-organization processes of molecular constituents are of a reversible dynamic nature driven by intermolecular forces such as hydrogen bonds, van der Waals forces, π-π stacking, and others [2]. The rational design of new gelators with promising groups for the formation of self-assembling structures is key to targeting materials with specific properties of interest [3]. Herein, isatin-derived semicarbazones are highlighted as promising gelling scaffold, benefiting from the hydrogen-bonding capability of the semicarbazone moiety and the anisotropic growth characteristics of the isatin core. Novel six isatin-based semicarbazones were synthesized via condensation reaction between*N*-alkyl (hexyl, dodecyl and hexadecane) isatins substituted at position 5 (5-H and 5-F) and semicarbazide. The reactions were carried out in ethanol using a catalytic amount of HCl, with reaction times ranging from 45 to 180 min and good yields (75-97%). The chemical structures were characterized by ^{1}H and ^{13}C NMR, IR and HRMS. All compounds formed stable gels in diesel, cyclohexane, cyclohexanol, ethylene glycol, propylene glycol, glycerol, and mineral oil, with minimum gelation concentration (MGC) as low as 0.4% (w/w). We found that the twelve-carbon alkyl chain at isatin in these semicarbazones formed a gel in a higher number of solvents, while the sixteen-carbon alkyl chain and fluorinated derivative showed the lower MGC in propylene glycol (Figure). The gels were also investigated using SEM and POM.



Chemical structures of all compounds and a photo of the gel 5c

Agradecimentos/Acknowledgments

UFPB, FAPESQ-PB, CAPES and CNPq for scholarships.

Mechanochemical Functionalization of Epoxides with Alcohols Catalyzed by $BiCl_3$

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Palavras Chave:*Mechanochemistry,catalysis,epoxides,alcohol*

Highlights

A green mechanochemical approach for $BiCl_3$-catalyzed epoxide ring opening with alcohols, achieving high conversions without solvents.

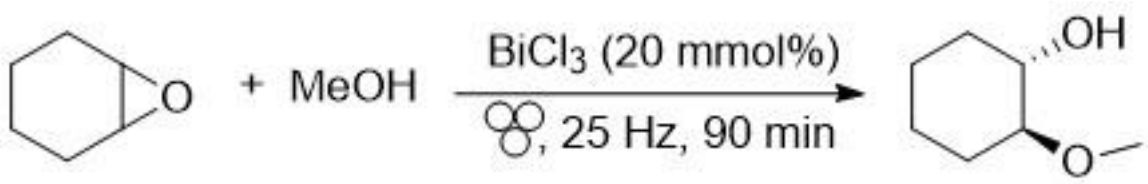
Resumo/Abstract

Mechanochemistry has emerged as a safe and energy-efficient technique, attracting interest in the optimization of organic reactions[1,2]. Epoxide ring opening is a valuable transformation, providing building blocks widely used in organic synthesis[3]. Previous studies employing europium-based catalysts showed unsatisfactory results in the functionalization of epoxides with alcohols, motivating the exploration of new catalytic species. In this work, the mechanochemical ring opening of epoxides with different alcohols catalyzed by bismuth chloride ($BiCl_3$) was investigated (Scheme 1). Initial experiments with methanol and cyclohexene oxide afforded conversions around 90%. Optimization using 20 mol% catalyst and 10 equivalents of methanol led to complete conversion, and the product was confirmed by mass spectrometry. Reactions with ethanol and 1-propanol also reached 100% conversion; in the latter case, two products were observed in a 58:42 ratio and are under investigation. The reaction with 1-butanol showed approximately 35% conversion.Epichlorohydrin was also evaluated with the same alcohols, affording conversions above 94%. A single product was obtained with methanol, whereas ethanol (90:10), 1-propanol (79:21), and 1-butanol (92:8) produced two products. The scope will be expanded to secondary and benzylic alcohols, as well as other epoxides such as 1,2-epoxybutane, 1,2-epoxyphenoxypropane, and styrene oxide, aiming to assess selectivity under the optimized conditions. Reactions proceed under mild and safe conditions, requiring up to 90 minutes of milling, highlighting the potential of mechanochemistry as a sustainable alternative for epoxide functionalization.

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Scheme 1 – Mechanochemical Ring Opening of Cyclohexene Oxide with Methanol

Agradecimentos/Acknowledgments

CAPES, CNPq, FACEPE, UFPE, CA-dQF, and DQO/SBQ

Metabolic Profiling of Coffea canephora Subjected to Controlled Fermentation with Saccharomyces cerevisiae

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Palavras Chave:*Fermentation,Metabolomics,Coffea canephora*

Highlights

Fermentation in coffee beans is a recent and emerging process. The study aims to conduct a metabolomic investigation of the fermentation process using different*Saccharomyces cerevisiae*strains.

Resumo/Abstract

Coffee is one of Brazil's most economically important agricultural products, and the market increasingly values specialty coffees with distinct sensory attributes and higher added value. Improvement processes, particularly controlled fermentation, have emerged as strategies to modulate the chemical profile of beans and consequently their sensory characteristics.
During coffee fermentation, microorganisms metabolize sugars and other mucilage compounds, generating metabolites that directly influence beverage quality. Understanding these chemical transformations is essential to make the process controllable and reproducible. In this context, metabolomics enables comprehensive profiling of metabolites formed during fermentation and supports correlations between process parameters and chemical changes in the beans.
This study aims to evaluate how fermentation parameters affect the chemical profile of Coffea canephora, contributing to the development of controlled and reproducible protocols with potential to enhance sensory quality. The experimental design comprises a factorial arrangement: 3 Saccharomyces cerevisiae strains × 1 C. canephora × 3 replicates × 1 additive × 3 fermentation times (72, 96, and 120 h). After fermentation, beans will be dried, ground, and subjected to metabolite extraction. Analyses will be performed by HPLC-MS and GC-MS to determine chemical variations under different conditions. Data processing will use MS-DIAL, MetaboAnalyst, GNPS2 and Sirius.
The study is ongoing. Preliminary chemical and sensory results indicate promising fermentation effects, with predominant production of organic acids associated with higher-quality coffees.
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Agradecimentos/Acknowledgments

Amanda H. N. would like to acknowledge the UNESP Chemistry Institute, the Department of Biochemistry and Organic Chemistry, Professor Dr. Alan Cesar Pilon, Project FAPESP/n°2025/24709-6, Project FAPESP n°15889-0, Project FAPESP 20/11967-3 and CNPq.

Metabolomic Evaluation of Cerrado Bacteria with Probiotic Properties by Nuclear Magnetic Resonance (NMR)

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Palavras Chave:*Cerrado Bacteria, NMR, metabolomics, IVDr*

Highlights

Standardized 1H NMR spectral processing (NMRProcFlow) enabled robust multivariate analysis across different instruments and experiments.

Resumo/Abstract

Integrated metabolomic approaches have revealed correlations between microbial composition and host metabolism. Byproducts of puçá and gabiroba showed prebiotic potential due to high fiber, lipid, and carbohydrate contents. To perform metabolomic characterization of probiotic microorganisms isolated from byproducts of native Brazilian Cerrado fruits, NMR experiments were conducted at 400 MHz (Bruker Avance I, FFCLRP-USP) using CPMG and NOESY pulse sequences. Samples were prepared with 540 µL of sample, 60 µL D_2O, and 20 µL TSP-d_4 in D_2O (100 mM). The same protocol was applied in collaborative experiments using a 600 MHz Bruker IVDr spectrometer (UFSCar). Spectral processing was performed using NMRProcFlow, including baseline correction, phase adjustment, TSP referencing, alignment, normalization, and binning (0.04 ppm). Data were exported to MetaboAnalyst for multivariate analysis. PCA revealed distinct and reproducible metabolic profiles. The filtered IVDr data showed greater replicate proximity and improved cluster definition, even with bucket-based analysis. Pediococcus acidilactici M7 (mangaba) and Weissella cibaria/confusa M1 (pequi peel) showed high similarity in multivariate space, forming consistent PCA clusters independent of instrumental conditions. Heatmap analysis confirmed the same increase and decrease patterns in the same buckets across all experiments and instruments. Metabolomic signatures indicate variability related to probiotic functionality, highlighting NMR metabolomics as an effective tool for screening microorganisms from Cerrado fruit byproducts. The workflow enables reliable metabolic profiling and supports applications in functional foods and health research.

Agradecimentos/Acknowledgments

The authors thank the Programa Unificado de Bolsas (PUB-USP) for the fellowship and CNPq, FAPESP, and FINEP for support to the NMR Laboratory, and acknowledge Prof. Antonio Gilberto Ferreira for access to the 600 MHz IVDr NMR equipment.

Methodological study of HPPD-inhibiting triketones synthesis from biomass-derived furoic acid

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Palavras Chave:*Triketones,Biomass,HPPD inhibitors,Furoic acid*

Highlights

In this work, a methodological study of a sustainable one-pot route was optimized to synthesize triketones herbicides using biomass-derived furoic acid as a renewable building block.

Resumo/Abstract

Food insecurity is one of the major challenges faced by society, primarily affecting countries in situations of socioeconomic vulnerability. Among the causes that intensify hunger, the presence of weeds in food crops reduces agricultural yield by competing with the main crop for environmental resources. The control of these weeds can be achieved using herbicides, chemical substances that interfere with the plants metabolic pathway and inhibit its growth. Therefore, the enzyme 4-hydroxyphenylpyruvate dioxygenase (HPPD) is considered an important biological target, as it is an essential enzyme in the plant metabolic process, and its inhibition can cause symptoms such as bleaching, necrosis, and death. Among the existing groups of herbicides, triketones stand out for their more selective inhibition of the HPPD enzyme compared to traditional herbicides. Thus, considering the need for developing more sustainable methods in organic synthesis, this project proposes the synthesis of new potentially HPPD-inhibiting compounds by substituting the phenyl group with a furan ring derived from furoic acid, a derivative obtained from renewable sources. A methodological study of a one-pot route was proposed, employing CDI as the coupling agent, in which the conditions were optimized and a yield of 81% was obtained. The success of the methodology validates the strategy for the development of new triketones with herbicidal potential and aligned with the principles of Green Chemistry.

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Development of new triketones herbicides using derivates of lignocelullosic biomass

Agradecimentos/Acknowledgments

The authors gratefully acknowledge FAPERJ, CNPq and CAPES for funding, as well as PPGQ-UFF.

Micellization Behavior and Critical Micelle Concentration of Novel Pyridinium-Based Ionic Liquids with Sulfonate Anions

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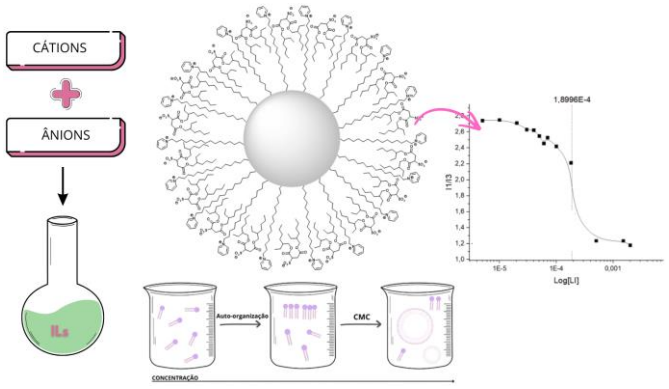
Palavras Chave:*pyridinium ionic liquids,micellar system,fluorescence probe*

Highlights

The critical micelle concentration of pyridinium-based ILs was determined by pyrene fluorescence spectroscopy. Alkyl chain branching and anion structure are show to directly control micellar.

Resumo/Abstract

The behavior of surfactant-like compounds in solution is strongly dependent on their concentration. In aqueous or mixed-solvent systems, increasing concentration leads to saturation of the liquid interface and to the onset of a characteristic point known as the critical micelle concentration (CMC). Above this point, excess molecules spontaneously self-assemble into supramolecular aggregates known as micelles. The CMC of ionic liquids (ILs) can be efficiently determined by fluorescence spectroscopy. The CMC of two novel pyridinium-based ILs bearing sulfonate anions was determined by fluorescence spectroscopy. Measurements were carried out in aqueous solutions containing a fixed pyrene concentration and increasing IL concentrations. The ratio between the intensities of the pyrene emission (I_1/I_3) was calculated and plotted as a function of surfactant concentration on a logarithmic scale, yielding sigmoidal curves. The CMC values were obtained from the inflection points after Boltzmann fitting, which correspond to micelle formation. The analysis of the I_1/I_3 ratio clearly evidenced the micellar transition and enabled correlation between the aggregation process and the structural features of the ILs. The branched system exhibited a CMC of 1.8 x 10^{-4} mol L^{-1}, whereas the system bearing linear alkyl chains and a benzenesulfonate anion showed a higher CMC (3.81 x 10^{-3} mol L^{-1}), which is associated with more efficient hydrophobic packing and the formation of more compact micelles. The presence of branching in the cation chain and the nature of the anion affected the CMC, indicating that geometric and electrostatic factors act cooperatively for micellar aggregation in aqueous solution. Thus, the results demonstrate that structural differences among the ILs, mainly the branching of the alkyl chain and the anion structure, directly contribute to the CMC values and hydrophobic packing efficiency, establishing a clear structure-aggregation relationship.



Obtaining CMC for fluorescence probe

Agradecimentos/Acknowledgments

The authors are grateful to Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPQ, Coordenação de Aperfeiçoamento Pessoal de Nível Superior (CAPES) for financial support.

Microwave-assisted lipase-catalyzed synthesis of endocannabinoid derivatives

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Palavras Chave:*Microwave,Recombinant lipase,Amidation,Esterification,Endocannabinoids*

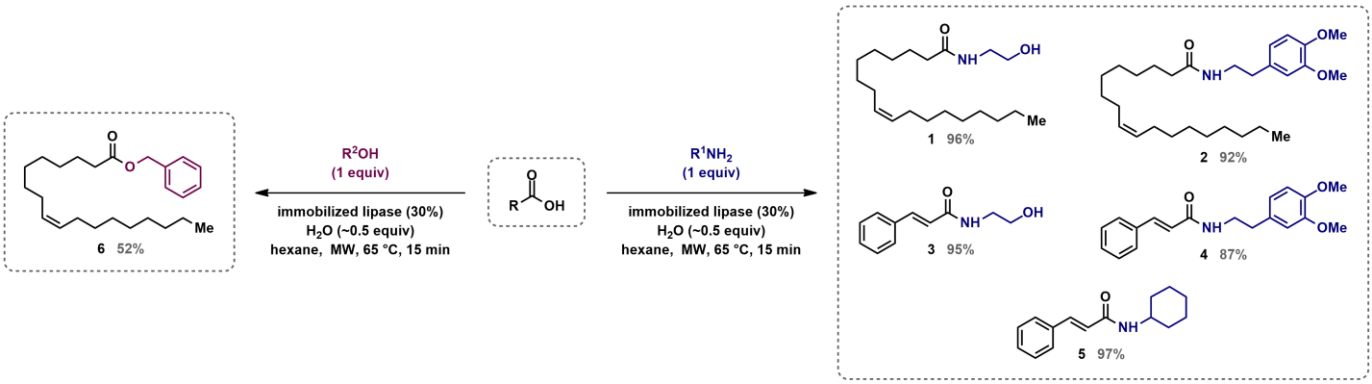
Highlights

Endocannabinoid derivatives were efficiently synthesized via microwave-assisted amidation and esterification reactions catalyzed by acrylic resin-immobilized lipase.

Resumo/Abstract

The endocannabinoid system plays a central role in physiological processes such as cognition, pain modulation, and immune response, and the development of ligands for its receptors (CB1 and CB2) is an important area of study in medicinal chemistry.[1] In this work, a microwave-assisted biocatalytic protocol was developed for the efficient preparation of endocannabinoid derivatives (**Scheme 1**), with further application in the synthesis of endogenous cannabinoids. Amidation and esterification reactions were carried out using an acrylic resin-immobilized lipase as the biocatalyst,[2] and the use of microwave (MW) heating allowed a significant reduction in reaction times.[3]Oleic acid was employed as a model compound for the optimization of reaction conditions (data not shown). Using the optimized conditions, the amidation reaction between oleic acid and ethanolamine in the presence of immobilized lipase (30% of the total mass of all reagents), under MW heating (65 °C) for 15 min, afforded oleoylethanolamide (OEA,**1**), an anandamide (AEA) derivative, in 96% isolated yield. Various combinations of carboxylic acids and amines were evaluated, affording compounds**2-5**in 87-97% isolated yields (**Scheme 1**). The same conditions were applied to the esterification of oleic acid with benzyl alcohol, providing benzyl oleate (**6**) in 52% isolated yield (**Scheme 1**). Further studies are underway to expand the scope of both amidation and esterification reactions.

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Scheme 1. Microwave-assisted enzymatic amidation and esterification reactions.

Agradecimentos/Acknowledgments

We are grateful to FAPESP and CNPq for the financial support. I.M.D. and K.R. thank CAPES for the scholarship.

Modulação de propriedades térmicas em cristais líquidos luminescentes derivados da unidade 5-metil-4,7-difenil-2,1,3-benzotiadiazol

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Palavras Chave:*Luminescência,Heterociclo,Mesofase*

Highlights

Ésteres derivados de 5-metil-4,7-difenil-2,1,3-benzotiadiazol, com diferentes cadeias alquílicas, foram sintetizados. As moléculas apresentaram absorção em 274 e 370 nm e emissão em 479 e 486 nm.

Resumo/Abstract

Os cristais líquidos são moléculas orgânicas constituídas por um núcleo aromático rígido ligado a longas cadeias flexíveis. Essa configuração confere anisometria e permite que a molécula apresente um estado intermediário entre o sólido e o líquido, no qual o material mantém a organização molecular, mas ainda exibe fluidez [1]. Essas substâncias são candidatas promissoras para uma ampla gama de aplicações optoeletrônicas [2].

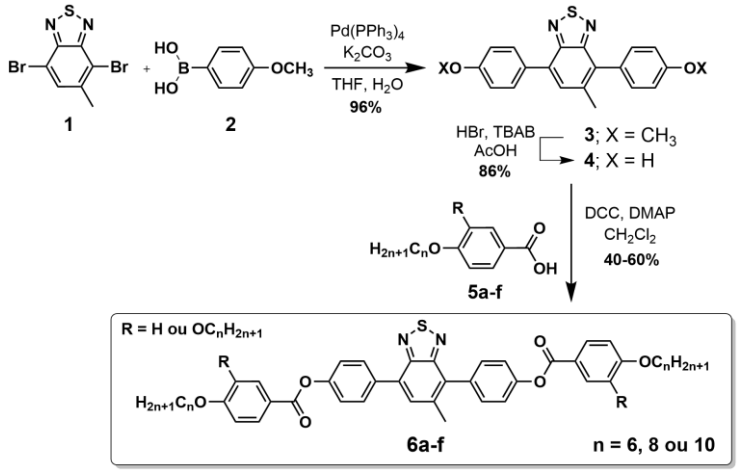
Neste trabalho, foi sintetizada e investigada uma série análoga composta por seis moléculas orgânicas derivadas do sistema 4,7-difenil-2,1,3-benzotiadiazol, contendo um substituinte lateral metila, visando à obtenção de cristais líquidos. A introdução do grupo metila busca reduzir as temperaturas de transição de fase.

A Figura 1 apresenta a rota sintética empregada para as moléculas finais. O rendimento das reações finais foi de 40-60%.

Foram empregados grupos éster como conectores entre o núcleo aromático e as diferentes cadeias flexíveis. Três das moléculas finais são dissubstituídas, com cadeias alquílicas lineares de 6, 8 e 10 átomos de carbono, enquanto as outras três são tetrassubstituídas. Essa estratégia permite avaliar, de forma comparativa, a influência do comprimento da cadeia e do grau de substituição sobre as propriedades ópticas e mesofases.

Em solução, os espectros de absorção no UV-Vis apresentaram bandas em 274 e 370 nm para todas as moléculas, indicando que as transições eletrônicas no estado fundamental são governadas pelo núcleo aromático central [3]. Por outro lado, os espectros de emissão apresentaram máximos em 479 e 486 nm, atribuídos aos ésteres com duas e quatro cadeias, respectivamente. Esses resultados sugerem que variações no padrão de substituição dos grupos periféricos podem influenciar as propriedades do estado excitado.

Análises de microscopia e de calorimetria devem evidenciar o impacto da substituição lateral nas temperaturas de transição.



Rota sintética dos compostos alvo.

Agradecimentos/Acknowledgments

UFBA, CNPq, CAPES.

New route for the preparation of a imino nitroxide organic radical with potential for use in solar cells

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Palavras Chave:*imino-nitroxides,organic radicals,organic photo collectors,organic solar cells*

Highlights

Imino nitroxide radicals show promise as photon collectors. A three-step synthesis of a radical molecule is described, with successful isolation and structural confirmation by X-ray diffraction.

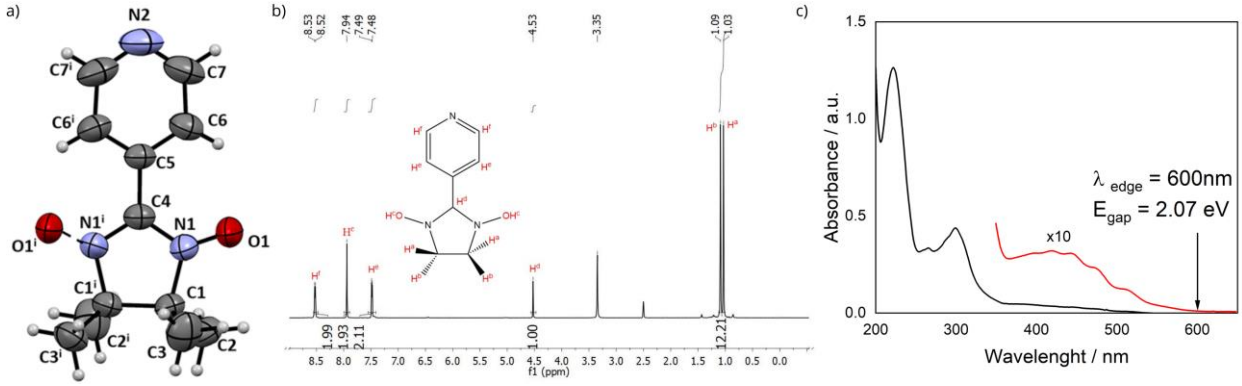
Resumo/Abstract

Organic solar cells are promising sustainable alternatives for energy conversion, aligned with the United Nations Sustainable Development Goals, particularly SDG 7. Within this framework, organic molecules with suitable electronic properties for photoexcitation are required. Stable organic radicals are attractive because they possess readily excitable unpaired electrons. Among them, imino nitroxide radicals combine high stability with favorable electronic structures arising from conjugated imine (C=N) and nitroxide (NO·) groups.

Herein, a novel three-step synthetic route to 4,4,5,5-tetramethyl-2-(pyridin-4-yl)iminonitroxide (p-RAI, Fig. 1a), starting from 2-nitropropane, is reported. Initially, 2,3-dimethyl-2,3-dinitrobutane (DNB) was prepared according to literature methods. Subsequently, partial reduction of DNB using NH_4Cl and zinc dust, followed by condensation with 4-pyridinecarboxaldehyde, was performed sequentially without isolation of the bis(hydroxylamine) intermediate, affording p-PBI (Fig. 1b) in 68% yield. This methodology enabled savings in time and reagents while maintaining yields comparable to conventional routes.

In the final step, p-PBI was oxidized to p-RAI using a new imino nitroxide oxidation protocol combining $NaNO_3$ and MnO_2 in methanol, alongside a catalytic amount of HCl. The target radical was obtained in 57% yield, representing a 31% increase compared to related procedures. Moreover, this route employs less toxic and lower-cost reagents, contributing to more sustainable synthetic practices.

The radical was characterized by infrared spectroscopy and single-crystal X-ray diffraction, and its crystal structure is reported here for the first time. It crystallizes in the same unit cell as its parental nitronyl radical, confirming that its stability is associated with steric shielding of the oxygen atoms. The compound exhibited an optical band gap of 2.07 eV and molar absorptivities of 275 and 3187 L mol^{-1} cm^{-1} at 415 and 300 nm, respectively.



a) Crystal structure of p-RAI b) 1H NMR spectrum for p-PBI c) UV–Vis absorption spectrum of p-RAI

Agradecimentos/Acknowledgments

We would like to thank CNPq (420443/2018-5), CAPES, and FAPEMIG (APQ-05311-23 and APQ-01948-22) for scholarships and financial support, LabCri for single crystal X-ray diffraction facilities and NEPs-DQ for all remaining characterization facilities.

New solvent-free mechanochemical methodology for synthesizing quinazolin-4(3H)-ones

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Palavras Chave:*Building blocks,N-Heterocyclic compounds,Mechanochemical methodology,Quinazolin-4(3H)-ones.,Quinazolin-4(3H)-ones*

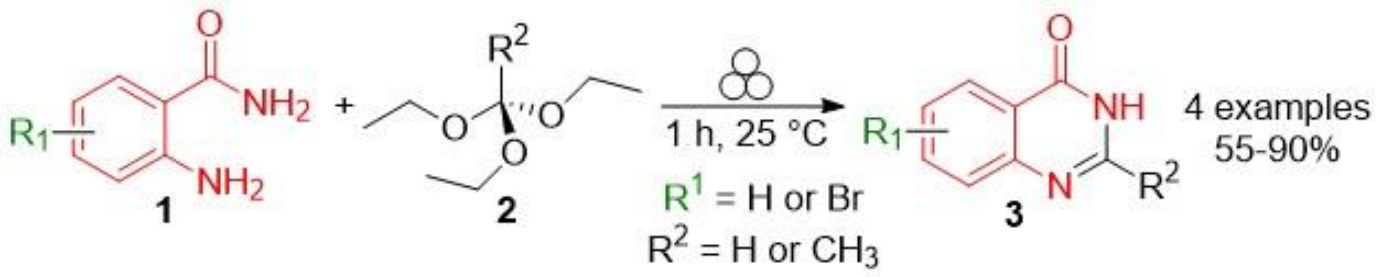
Highlights

Quinazolin-4(3*H*)-ones are privileged compounds in medicinal chemistry. Mechanochemistry is an important tool in the search for more sustainable synthetic methodologies.

Resumo/Abstract

Quinazolin-4(3*H*)-ones play an important role in medicinal chemistry due to their remarkable biological and pharmacological properties. Furthermore, these*N*-heterocyclic compounds are important building blocks for 4-anilinoquinazolines, which are prevalent structures in anticancer compounds.[1] Thus, to develop a more environmentally friendly methodology to synthesize quinazolin-4(3*H*)-ones from 2-aminobenzamides, in this work, we have been investigating a solvent-free methodology to perform the cyclocondensation between 2-aminobenzamides and different orthoesthers. Initially, we tried to replicate a methodology previously described in the literature,[2] but even by increasing the reaction time, we were unable to obtain the reported yields. Thus, to overcome these problems, we investigated the reaction between 2-aminobenzamide (**1**) and triethyl orthoformate (**2**) using TFA as a catalyst under mechanochemical conditions. After some tests, we achieved the full conversion (via GC-FID) of the starting material into product using a milling frequency of 25 Hz for 1.0 h at 25 °C, resulting in quinazolinone**3**in 90% yield (Scheme 1). In sequence, using substituted 2-aminobenzamides and different orthoesthers, we can obtain three more quinazolinones of type**3**in yields ranging from 55-87%.
In summary, we developed a new solvent-free methodology for synthesizing quinazolin-4(3*H*)-ones of type**3**, which has proven to be a promising alternative for the synthesis of these important*N*-heterocyclic compounds. Therefore, to assess the scope of this methodology, further studies are currently being conducted in our research group.

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Scheme 1

Agradecimentos/Acknowledgments

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Novel β-Carboline–bithiophene Hybrids: Synthesis and Antileishmanial Activity

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Palavras Chave:*Synthesis β-Carboline–bithiophene; Antileishmanial Activity*

Highlights

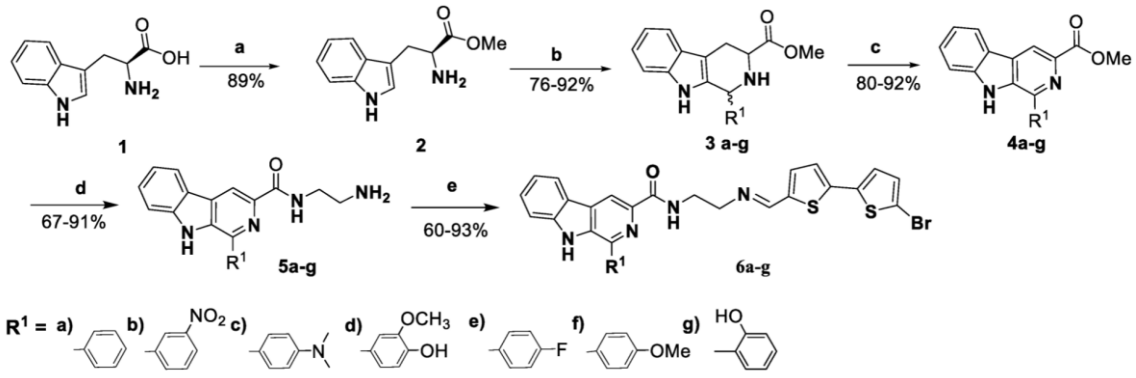
β-Carboline–bithiophene hybrids were synthesized and evaluated against Leishmania amazonensis. Most active compound showed IC_{50} of 6.17 µM and selectivity index of 12 toward amastigotes.

Resumo/Abstract

Leishmaniasis is a neglected parasitic disease caused by*Leishmania*spp. and remains endemic in 99 countries, affecting approximately 12 million people worldwide. Current treatments are limited by drug toxicity, prolonged regimens, and increasing parasite resistance, highlighting the need for safer and more effective antileishmanial agents [1]. The β-carboline nucleus has emerged as a privileged scaffold for the development of novel antileishmanial compounds [2]. To obtain novel antileishmanial compounds, this study explored the molecular hybridization of the β-carboline nucleus with a bithiophene moiety, known to exhibit a broad spectrum of biological activities, including antileishmanial effects [3]. Thus, a series of β- carboline-bithiophene hybrids (**6a-g**) were synthesized (Scheme 1) and evaluated against*Leishmania amazonensis*. Carboxamides**5a-g**were obtained from the Pictet-Spengler condensation of L-tryptophan methyl ester (**2**) with aldehydes, oxidation of**3a-g**, and reaction of the β-carbolines**4a-g**with ethylenediamine. The Schiff bases**6a-g**were prepared from the condensation of 5a-g with 5′-bromo-2,2′-bithiophene-5-carboxaldehyde. The assays results showed that, except for**6b**, the compounds were more active against amastigotes than promastigotes, with IC_{50} values ranging from 6.17 to 35.45 µM. The most active compound,**6g**, exhibited an IC_{50} of 6.17 µM against intracellular amastigotes and a good selectivity index (SI), being 12-fold more toxic to*L. amazonensis*amastigotes than to J774-A1 mammalian cells. The reference drug used (miltefosine) exhibited IC_{50} of 1.75 µM and SI of 31 towards amastigotes. Our results demonstrate the antileishmanial activity of β-carboline–bithiophene hybrids, evidencing the potential of this scaffold for further studies.

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Reagents and Conditions: a) CH_3OH, H_2SO_4, reflux, 48 h; **b)** RCHO, CH_2Cl_2, TFA, t.a, 48 h, **c)** S, xylene, reflux, 48 h; **d)** ethylenediamine, ta, 24 h; **e)** 5'-bromo-2,2'-bithiophene-5-carboxaldehyde, EtOH, reflux, 20 h.

Scheme 1. Synthetic route for compounds **6a-g**

Scheme 1. Synthetic route for compounds 6a-g

Agradecimentos/Acknowledgments

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On the Mechanism of Ketene Three-Component Reaction

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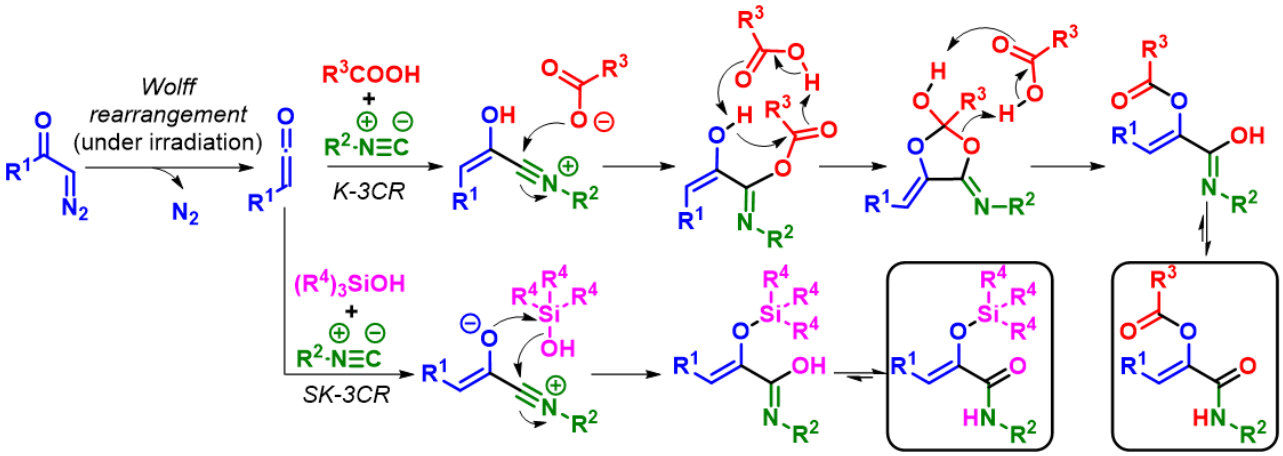
Palavras Chave:*Multicomponent Reaction,Ketene,Rearrangement,Mechanism,DFT*

Highlights

The mechanism involved in the Silylative-Ketene and Ketene three-component reactions was investigated by mass spectrometry and DFT calculations, revealing distinct pathways for each transformation.

Resumo/Abstract

Multicomponent reactions (MCRs) are an important class of transformations due to the rapid construction of structurally complex molecules from reactions involving three or more components, minimizing purification steps and providing high atom economy. Among the MCRs, the ketene three-component reaction (K-3CR) and its silylative variant (SK-3CR) are transformations involving α-diazoketones (*in situ*converted into ketenes by Wolff rearrangement), isocyanides, and carboxylic acids (for K-3CR) or silanols (for SK-3CR) and constitute powerful strategies for the synthesis of α-acyloxy- and α-silyloxyacrylamides, motifs commonly encountered in bioactive molecules and valuable as versatile synthetic building blocks. Although these reactions are experimentally straightforward, reliable, and broadly useful, several fundamental aspects of their reaction pathways have not been fully clarified. Based on our experience in MCR mechanistic investigations, a combined density functional theory (DFT) calculation and mass spectrometric reaction monitoring study was carried out. Our findings suggested that, although similar transformations, the reaction pathway is distinct for each one (Scheme 1). For K-3CR, due to the presence of carboxylic acid and its ability to mediate proton-transfer steps, a Passerini-like mechanism was identified as more plausible, involving the Mumm rearrangement as the key step. On the other hand, due to the weak proton-shuttle ability of silanols, as well as steric and electronic effects, the reaction pathway involves a direct transfer of the silyl group. This approach enables a coherent description of the complete reaction landscapes for both processes, identifying key intermediates, elementary steps, and the mechanistic bifurcation distinguishing the two pathways, highlighting the efficiency of the integration of these tools in mechanistic investigations.



Scheme 1. Plausible mechanisms for K-3CR and SK-3CR.

Agradecimentos/Acknowledgments

The authors are grateful for the generous financial support from CAPES, UFJF, FAPEMIG, and CNPq.

OXIDATIVE COUPLING SYNTHETIC METODOLOGY FOR OBTAINING DICYANOSTYLBENES, PORPHYRAZINE KEY PRECURSORS, USING PHASE TRANSFER CATALYSIS

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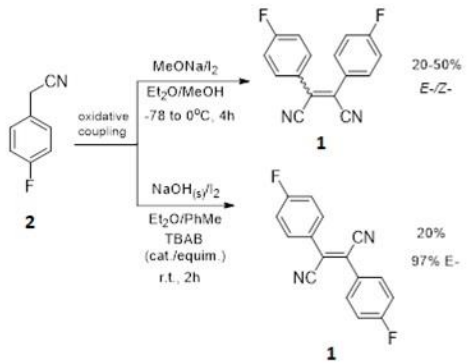
Palavras Chave:*Alpha,beta-dicyano-4,4'-difluorstylbene,4-Fluoracetonitrile,Oxidative Coupling,Solid Phase Transfer Catalysis*

Highlights

Phase Transfer Catalysis can be promising and efficient synthetic methodology for obtaining α,β-dicyanostilbenes, key precursors for corresponding porphyrazines with important biological applications

Resumo/Abstract

Nowadays, α,β-dicyanostilbenes draw great attention as key building blocks for the synthesis of tetraazaporphyrins (TAPs), promising fluorescent agents for Photodynamic Therapy [1] and as intelligent photo-responsive materials. These compounds have been generally prepared from phenylacetonitrile derivatives by oxidative coupling reaction with iodine and alkoxide in anhydrous solvent, as described by Knoevenagel [3]. In fact, this reaction mechanism might be similar to that of iodoform, but monoiodination may be selective with low temperature (-78 oC - 0 oC) and very controlled reagent addition. Nevertheless, higher base concentrations are needed, leading to side reactions that culminate in diiodination, formation of maleimide and subsequent polymerization, resulting in low to modest reaction yields (**Scheme 1**) with low stereoselectivity [4,5]. This selective monoiodination and dimerization processes can be performed under milder conditions. Phase Transfer catalysis (PTC) is a very well-known synthesis methodology [6] for accelerating and improving yields of reactions, specially for replacing strong and expensive organic bases as alkoxides with cheaper and safer inorganic bases (NaOH, K_2CO_3, etc…), which is also essential for "green chemistry" principles. The present work shows the preliminary investigation for obtaining α,β-dicyano-4,4'-difluorstilbene (4-F-C_6H_4-C(CN)=C(CN)-4'-F-C_6H_4,**1**), starting from 4-fluophenylacetonitrile (**2**) using PTC solid-liquid conditions (NaOH(s), 2:1 mol/mol; Bu_4NBr, 10-100%, iodine-1:1 mol/mol, 2h) in organic solvents (diethyl ether/toluene) and magnetic stirring at room temperature. After several experiments using different reaction conditions, similar product yields could be achieved, but with higher selectivity of the E-isomer (97%) and with more efficiency and reproducibility. It can be concluded that the PTC methodology can really be a promising and easier alternative for obtaining α,β-dicyanostilbenes.



Scheme 1. Comparison between conventional and PTC solid-liquid synthetic methodologies for the preparation of α,β-dicyano-4,4'-difluorstilbene (**1**) from 4-fluophenyl acetonitrile (**2**)

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Agradecimentos/Acknowledgments

CNPq, FAPEMIG, DQ-UFMG

Photocatalyst-Free, Blue LED-Mediated Multicomponent Strategy for the Synthesis of 5-Amino-4-Chalcogenyl-1H-Pyrazoles

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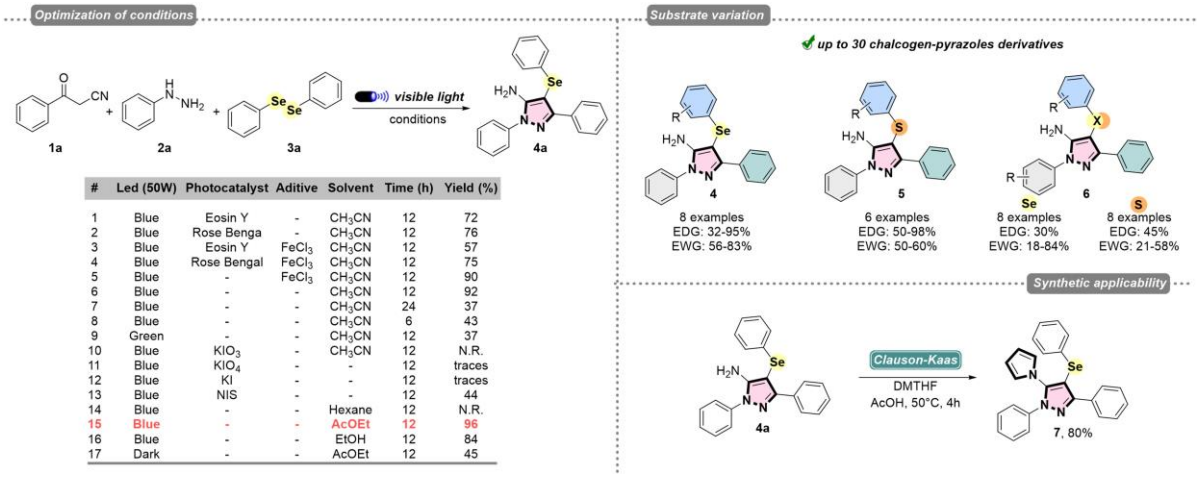
Palavras Chave:*Development of a mild, visible-light-driven, photocatalyst-free multicomponent protocol for chalcogen-functionalized pyrazoles.,Heterocycles, selenium, multicomponent, visible-light,Heterocycles, chalcogen, multicomponent, visible-light*

Highlights

Development of a mild, visible-light-driven, photocatalyst-free multicomponent protocol for chalcogen-functionalized pyrazoles.

Resumo/Abstract

Pyrazole derivatives are an important class of heterocycles with broad applications in medicinal chemistry, materials science, and catalysis due to their unique electronic structure and versatile functionalization.[1] The introduction of chalcogen elements into heterocyclic frameworks is an efficient strategy to modulate molecular properties, benefiting from the high polarizability and directional noncovalent interactions of sulfur and selenium. In this work, we report a mild, multicomponent, visible-light-driven and photocatalyst-free approach for the synthesis of chalcogen-containing pyrazoles.[2] Initially, the reaction conditions were carefully optimized by systematically varying the light source, irradiation power, photocatalyst, additives, reaction time, temperature, solvent, and iodine source. This study revealed that the best performance was achieved under additive- and photocatalyst-free conditions using catalytic iodine under blue LED irradiation (50 W) for 12 h in ethyl acetate as a greener solvent. With the optimal conditions in hand, the substrate scope was then expanded to a broad range of diselenides and disulfides, as well as diverse hydrazines, enabling the synthesis of more than 30 structurally diverse chalcogenated pyrazole derivatives. Finally, the synthetic utility of the method was demonstrated through derivatization of the main product via a Clauson-Kaas reaction, providing access to more complex molecular architectures. This operationally simple approach delivers structural diversity and improved sustainability, representing an efficient platform for accessing functional chalcogenated pyrazoles with potential applications in medicinal and materials chemistry. References: 1)Moussa et al.,*Heliyon*, 2024, 10 (20), e38894.; 2)Ángel et al.,*Molecules*, 2023, 28 (7), 3056.



#	Led (50W)	Photocatalyst	Aditive	Solvent	Time (h)	Yield (%)
1	Blue	Eosin Y	-	CH_3CN	12	72
2	Blue	Rose Benga	-	CH_3CN	12	76
3	Blue	Eosin Y	$FeCl_3$	CH_3CN	12	57
4	Blue	Rose Bengal	$FeCl_3$	CH_3CN	12	75
5	Blue	-	$FeCl_3$	CH_3CN	12	90
6	Blue	-	-	CH_3CN	12	92
7	Blue	-	-	CH_3CN	24	37
8	Blue	-	-	CH_3CN	6	43
9	Green	-	-	CH_3CN	12	37
10	Blue	KIO_3	-	CH_3CN	12	N.R.
11	Blue	KIO_4	-	-	12	traces
12	Blue	KI	-	-	12	traces
13	Blue	NIS	-	-	12	44
14	Blue	-	-	Hexane	12	N.R.
15	Blue	-	-	AcOEt	12	96
16	Blue	-	-	EtOH	12	84
17	Dark	-	-	AcOEt	12	45

Synthesis of 4-arylchacogenyl-1H-pyrazoles.

Agradecimentos/Acknowledgments

UFSC, UFF, CNPq, CAPES, FAPERJ.

Phthalides analogues resulting from Diels-Alder reaction characterized by NMR analyses and DFT calculations

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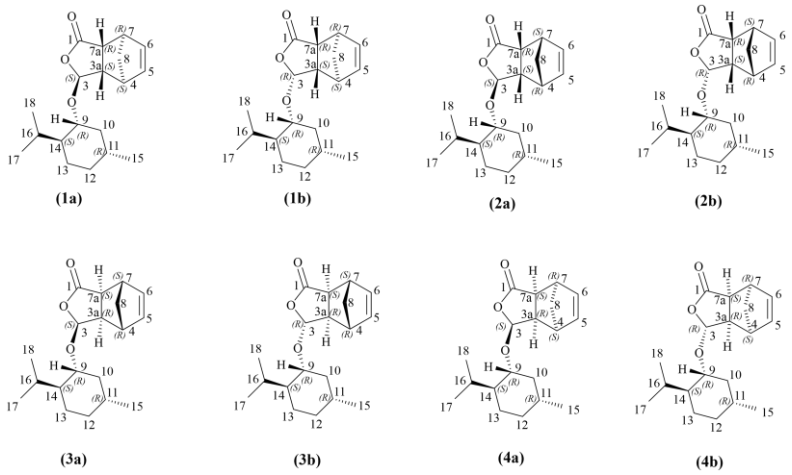
Palavras Chave:*Isobenzofuranones,Diels-Alder reaction,theoretical calculations,VCD.,VCD*

Highlights

Synthesis and structural elucidation of phtalides analogs by Diels-Alder reaction. Use of theoretical calculations for structural confirmation.

Resumo/Abstract

Isobenzofuranones, also known as phthalides, are bicyclic compounds widely found in both natural and synthetic products and exhibit diverse biological activities, including anti-inflammatory, antitumor, antioxidant, and pesticidal properties. In the synthesis of new phthalide analogues, the Diels-Alder (DA) reaction represents an efficient synthetic strategy, combining excellent atom economy with the ability to generate up to four stereogenic centers in a single step. In this study, the Diels–Alder reaction between cyclopentadiene and (5*S*)-5-((2-isopropyl-5-methylcyclohexyl)oxy)furan-2(5*H*)-one was investigated, aiming to obtain and characterize adducts arising from endo and exo orientations combined with syn and anti positions of the diene relative to the substituent (Figure, compounds 1a to 4b). The products were isolated by column chromatography and characterized by NMR spectroscopy, supported by DFT calculations. The observed stereoselectivity was attributed to secondary orbital interactions and steric effects. To determine the absolute configuration of the chiral centers, Vibrational Circular Dichroism (VCD) analyses were performed by comparing experimental data with theoretical spectra obtained at the B3LYP/PCM($CDCl_3$)/6-31G(d,p) level. This study contributes to a deeper understanding of stereoselectivity in Diels–Alder reactions involving chiral lactones and supports the development of synthetic strategies for obtaining functionalized phthalides.



Structures of adducts 1a-4b

Agradecimentos/Acknowledgments

FAPEMIG, CNPq, CAPES, UFV

Pillararenes as nanoreactors applicable to photochemical reactions of heterocycles

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Palavras Chave:*Macrocycles,pillararenes,photochemistry,heterocycles,fluorescence*

Highlights

Synthesis and photophysics of Imidazole-functionalized pillar[5]arene.

Host–guest binding with uracil predicted by molecular docking.

Potential nanoreactor for [2+2] photocycloaddition.

Resumo/Abstract

Pillararenes are a class of macromolecules first synthesized by Ogoshi in 2008 and widely explored in supramolecular chemistry. Due to the multiple noncovalent interactions established inside and outside the macrocycle, these species act as host–guest systems, promoting the encapsulation of linear and aromatic ligands. This complexation enables pillararenes to mimic biological systems, such as enzymes, by positioning substrates in a manner favorable to reaction occurrence. This architecture allows their function as nanoreactors favoring, for example, photodimerizations that would hardly occur in the absence of spatial restriction.[1,2]

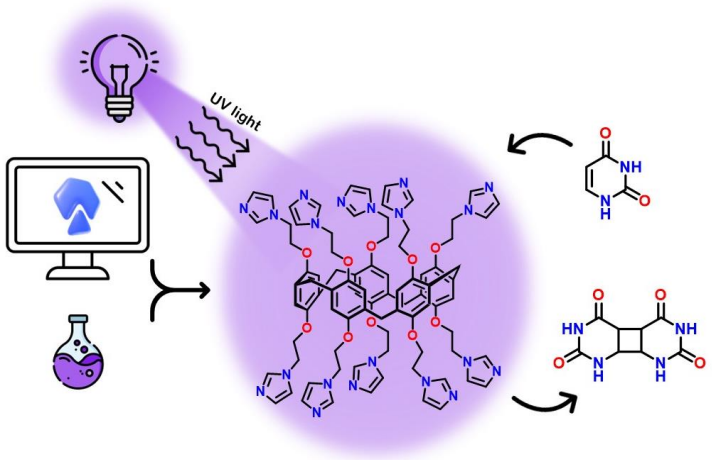
Based on these properties, computational simulations were performed using different molecular docking methodologies to predict the interactions between an imidazole-functionalized pillar[5]arene (receptor) and one or two uracil molecules and its dimer (substrates), evaluating the probability of encapsulation before and after the [2+2] cycloaddition. The simulations indicated affinity between receptor and substrate, with free energies ranging from –7.00 to –2.44 kcal/mol, mainly attributed to hydrogen bonds between the uracil hydrogens and the oxygen atoms of the macrocycle, with average distances of approximately 2.4 Å.

The pillar[5]arene was synthesized via a tosylated intermediate with a yield of 65%. Photophysical studies of the commercial heterocycle and the receptor were conducted in different solvents, evaluating fluorescence and conformational rigidity in distinct chemical environments and in their mutual presence. Absorption bands at wavelengths of 256 and 293 nm (substrate and receptor) and fluorescence emission bands at 338 and 322 nm were analyzed. Notably, pillar[5]arene fluorescence was observed for the first time in this work, representing an important property for supramolecular photochemistry.

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[1] ACS Omega 2026, 11, 1849−1866.

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Scheme of the synthetic and theoretical photochemical process of pillar[5]arene–heterocycle system.

Agradecimentos/Acknowledgments

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Polyhydroxyalkanoates (PHA)s from Azospirillum brasilense under different nutritional conditions.

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Palavras Chave:*Polyhydroxyalkanoates (PHAs), Azospirillum brasilense, Biopolymers.*

Highlights

*Azospirillum brasilense*showed potential for PHA production.

Among the media tested, molasses at a C/N ratio of 60:1 stood out in PHA production.

Resumo/Abstract

Polyhydroxyalkanoates (PHAs) are biodegradable and biocompatible polymers, accumulated by microorganisms as an intracellular reserve of carbon and energy, and stand out as sustainable alternatives to petrochemical-derived polymers[1]. In this work, the production of PHAs by*A. brasilense*strains in different culture media was evaluated. The strains were maintained in YMA (Yeast Mannitol Agar) medium, and propagation was carried out from fresh colonies cultivated for 24 h at 30 °C, under orbital shaking at 180 rpm, in liquid YM (Yeast Mannitol) medium. The culture media were formulated by varying the carbon sources (glucose, sucrose, palm oil, and molasses), nitrogen sources (sodium nitrate and urea), and combined in carbon/nitrogen ratios (C/N = 20:1, 40:1, 60:1). Biomass production was used as an initial criterion for selecting the most promising conditions. PHA was extracted from dry biomass by digestion with concentrated H_2SO_4, followed by analysis at 235 nm (conversion of the polymer to crotonic acid)[2]. The best yield was obtained in the medium with molasses, C/N 60:1, with a total dry mass of 9.40 g and a production of 1.65 g of PHA (17.54% cellular biomass). In contrast, the lowest yield was observed in the media with glucose at a C/N ratio of 20:1, which showed low biomass values and a PHA yield of less than 5% of the dry biomass. The study highlights the potential of*A. brasilense*as a PHA producer. It reinforces the viability of using lower-cost substrates, contributing to the development of more economically viable processes for biopolymer production.

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Agradecimentos/Acknowledgments

*Azospirillum brasilense*showed potential for PHA production.

The composition of the medium and the C/N ratio influenced polymer yield production.

Among the media tested, molasses at a C/N ratio of 60:1 stood out in PHA production.

Preparation of Organoselenium Isoxazole Derivatives via TCCA-Activated Diselenides

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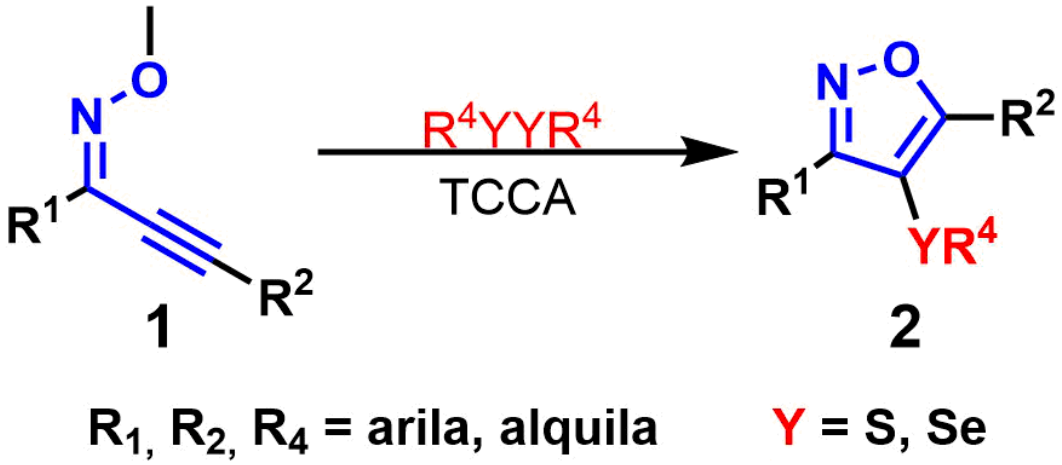
Palavras Chave:*Isoxazoles, organoselenium compounds, selenylation, TCCA, cyclization*

Highlights

Nitrogen heterocycles in important motifs in chemistry. Using TCCA and diselenides, we developed an efficient selenylation–cyclization method. Selenylated isoxazoles were synthesized in high yields.

Resumo/Abstract

Nitrogen-based heterocycles are fundamentally important in both pharmaceutical and chemical research. A particularly relevant scaffold is the isoxazole ring, which features prominently in a variety of bioactive molecules, therapeutic drugs, and agrochemicals like pesticides.
In parallel, organoselenium compounds have become a focus of considerable scientific attention because of their versatile properties. Within pharmacology, the incorporation of selenium is linked to an array of biological effects, such as anti-Alzheimer, antiviral, antidepressant, and antioxidant activities.
More recently, methodologies employing trichloroisocyanuric acid (TCCA) in ethanol, combined with diselenides, have proven effective for conducting selenylation reactions and forming heterocyclic systems via cyclization. Therefore, we explored the use of this approach to synthezise selenylated isoxazoles, culminating in a synthetic procedure that allowed the synthesis of 7 selenylated isoxazoles, with yields up to 95%.



General outline of the synthetic methodology.

Agradecimentos/Acknowledgments

The authors thank FAPESC, CAPES, CNPq and INCT Catalise for the financial support as well as Universidade Federal de Santa Catarina for the institutional support.

PURIFICATION DEVELOPMENT OF SYNTHETIC CANNABIDIOL FOR FORCED-DEGRADATION STUDIES

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Palavras Chave:*Cannabidiol,Crystallization,Purification*

Highlights

Study of the purification of synthetic cannabidiol (CBD) under different conditions to obtain a high-purity product suitable for degradation testing.

Resumo/Abstract

Introduction:*Cannabis sativa'*seffects are primarily attributed to cannabidiol (CBD)[1], which offers high therapeutic potential for chronic pain and anxiety without psychoactive effects.[2] Establishing commercial viability requires forced degradation studies to define stability and storage parameters. Crystallization is a critical purification step, achieving ultra-high purity is fundamental to guarantee the efficacy and safety of the Active Pharmaceutical Ingredient (API).

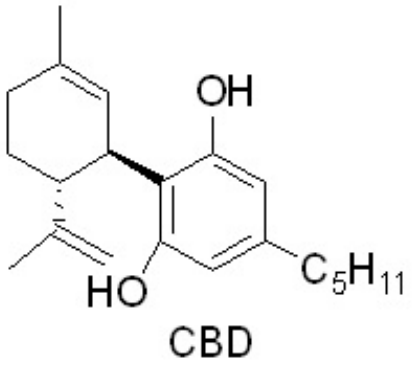
Objective: To synthesize CBD via a hybrid route (continuous-flow/batch) and optimize successive purification and crystallization processes to reach a ≥99.99% purity standard, complying with RDC 318/2019 for forced degradation studies.

Methodology:CBD was synthesized via a two-step route integrating continuous-flow and batch conditions[3]. The crude product underwent purification using various solvent systems (MeOH/*n*-heptane; MeOH:H_2O 90:10 with isooctane; and MeOH:H_2O 90:10 with*n*-heptane), followed by silica plug filtration. Finally, CBD was crystallized in*n*-heptane at -10 °C[4] and washed with*n*-heptane or isooctane.

Results: Post-synthesis, CBD was obtained as a dark viscous oil (74% purity). To meet the 99.9% threshold required for degradation studies, successive purifications were performed. Initial steps raised purity to 83%, and subsequent silica treatment reached 90%. Crystallization in*n*-heptane at -10 °C further increased this to 99.5%. However, this remains below the 99.99% pharmacopeial specification for the API, necessitating further optimization.

Conclusion: Although crystallization significantly improved purity, it did not meet RDC 318/2019 criteria for stability testing[5]. Additional crystallization experiments and pre-purification studies are required to meet regulatory standards.

References:1. Bonini et al. 2018; 2. Hanuš et al. 2016; 3. Braga et al. 2024; 4. Bonilla et al. 2025; 5. ANVISA RDC 318/2019.



Structure of Cannabidiol

Agradecimentos/Acknowledgments

The authors thank the Institute of Chemistry of the Federal University of Rio de Janeiro (IQ-UFRJ) and the funding agencies CNPq and CAPES for financing the research.

Rapid Enantiomer Quantification by ^{13}C NMR (3-14 min): A Miniaturized Method with Reduced Chiral Derivatizing Agent Consumption

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Palavras Chave:*chiral derivation agentacquisition parameters,nmrprocflow,enantiomeric quantification,chiral derivation agent,acquisition parameters*

Highlights

Fast miniaturized ^{13}C NMR method enables accurate enantiomer quantification using less (S)-citronellal and fewer scans, reducing acquisition time while maintaining analytical reliability.

Resumo/Abstract

Despite the successful use of (S)-citronellal as a chiral derivatizing agent (CDA) for the determination of the enantiomeric excess (ee) of primary amines by NMR, it remains essentially the only reported linear terpene aldehyde used for this purpose, even after years. Furthermore, previous studies have not systematically evaluated key quantitative NMR parameters, such as relaxation time (D1) and the number of scans (NS). Typical quantitative ^{13}C NMR conditions were employed (~1500 scans), resulting in relatively long acquisition times.

In this study, we investigated whether reliable ee quantification could still be achieved under significantly faster conditions, using NS values commonly associated with ^{1}H NMR experiments (64 and 128 scans) combined with shorter relaxation times (D1 = 2–5 s). Additionally, we evaluated the miniaturization of the method with a shorter acquisition time and CDA consumption.

The experiments were initially performed using 20 µL of (S)-citronellal and the chiral amine sec-butyl, following the protocol and varying the D1 and NS values. Subsequently, the CDA volume was reduced to 10 µL to assess whether a lower reagent consumption would still provide accurate enantiomeric quantification in racemic mixtures. Samples were prepared in quintuplicate and each was measured three times by NMR to ensure the reproducibility of the results.

The derivatization procedure followed the reported protocol and the NMR spectra were acquired on a 9.4 T spectrometer (100 MHz for ^{13}C NMR), using a Bruker Avance I instrument (5 mm Dual $^{13}C/^{1}H$ Z3756/0186 probe), with the acquisition parameters systematically varied (Table 1).

Therefore, the spectra were processed and quantified at (https://nmrprocflow.org), with the results showing excellent agreement with the theoretical values, demonstrating how the proposed approach allows for reliable quantification of enantiomers in faster acquisitions with lower CDA consumption and with robust and reproducible processing.

Table 1. Effect of CDA Volume and ^{13}C NMR Acquisition Parameters (D1 and NS) on Enantiomeric Quantification

CDA Volume	D1	NS	AQ	*S,S*	*S,R*	DESVPAD
20 uL	2	64	1,366	50,28	49,72	0,19
20 uL	2	128	1,366	50,02	49,98	0,01
20 uL	5	64	1,366	49,99	50,01	0,00
20 uL	5	128	1,366	50,16	49,84	0,11
CDA Volume	**D1**	**NS**	**AQ**	***S,S***	***S,R***	**DESVPAD**
10 uL	2	64	1,366	49,22	50,78	0,55
10 uL	2	128	1,366	50,59	49,41	0,41
10 uL	5	64	1,366	51,12	48,88	0,79

Effect of CDA Volume and ^{13}C NMR Acquisition Parameters (D1 and NS) on Enantiomeric Quantification

Agradecimentos/Acknowledgments

The authors thank the Programa Unificado de Bolsas (PUB-USP) for the fellowship and CNPq, FAPESP, and FINEP for the continuous financial support and infrastructure provided to the NMR Laboratory.

Reações Fotomediadas na Síntese de 4-(calcogenil)-1H-isocromen-1-onas com Potencial Farmacológico

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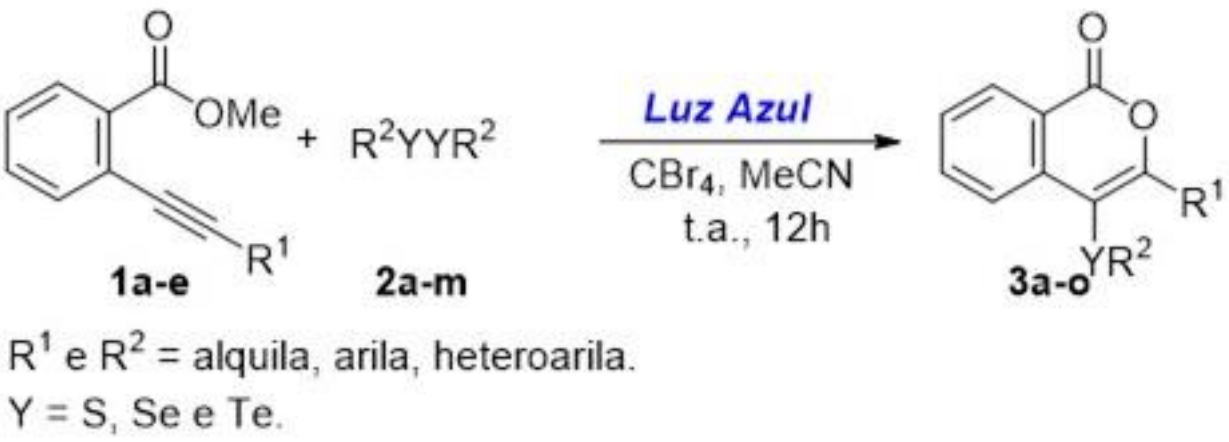
Palavras Chave:*Fotoquimica,Cromenonas,Organocalcogênios,Química Sustentável,Selênio*

Highlights

Visible-light-mediated photoreactions enable the sustainable synthesis of 4-(chalcogenyl)-1H-isocromen-1-ones with selective S/Se/Te incorporation and pharmacological potential.

Resumo/Abstract

As reações fotoquímicas orgânicas mediadas por luz visível têm se consolidado como ferramentas eficientes e sustentáveis na síntese orgânica, possibilitando transformações químicas sob condições brandas e com reduzido impacto ambiental. Nesse contexto, metodologias fotomediadas livres de fotocatalisadores destacam-se do ponto de vista da Química Verde, uma vez que minimizam o uso de insumos, simplificam os processos de purificação e operam com fontes de luz de baixa energia.
Neste trabalho, apresentamos o desenvolvimento de uma metodologia fotoquímica sustentável para a síntese de 4-(calcogenil)-1H-isocromen-1-onas a partir de 2-alquinil ésteres e dicalcogenetos de diorganoíla, utilizando tetrabrometo de carbono (CBr_4) como mediador sob irradiação de luz visível. A estratégia baseia-se na geração*in situ*de espécies eletrofílicas de calcogênio, que promovem a adição seletiva ao sistema alquinílico, seguida de ciclização intramolecular, conduzindo de forma eficiente à formação do núcleo isocromenona. Os compostos obtidos apresentam potencial interesse farmacológico, uma vez que são planejados com base no conceito de hibridização molecular, combinando em uma única estrutura o núcleo isocromenona e unidades calcogeniladas, ambos reconhecidos como motivos estruturais relevantes em moléculas bioativas.



Síntese Fotoinduzida de 4-(calcogenil)-1H-isocromen-1-onas

Agradecimentos/Acknowledgments

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Rotovibrational infrared spectrum analysis of organofluorine compounds in the gas phase.

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Palavras Chave:*infrared,gas phase,organofluorine compounds*

Highlights

The biohysterism between C–F, C–H, and C–O bonds arises from similar van der Waals radii (1.20, 1.52, and 1.47 Å), yet organofluorines show distinct reactivity, stability, and conformations.

Resumo/Abstract

Substituted fluorophenols at the ortho, meta, and para positions have been widely studied with emphasis on syn and anti-conformers. For 2-fluorophenol, the deviation of the H–O–C and C–F bond axes bring the atoms closer, enabling an intramolecular hydrogen bond. [1–7]

In the liquid phase, fluorophenols form associated polymeric species, hindering conformer band resolution; at high concentrations, broad and poorly defined bands lead to loss of conformational information. Gas-phase analysis at low concentration minimizes intermolecular association, providing favorable conditions for conformational studies. Two conformers are expected to appear in the O-H region; however, it is possible to detect the appearance of 3 bands (Figure 1), at different temperatures and different resolutions. Theoretical studies are investigating the origin of these bands (pure O-H, or interactions with syn with fluorine). Once determined, this study is going to be expanded to higher concentration analysis and the influence on the formation of these bands. Considering, now, the rotational spectrum.

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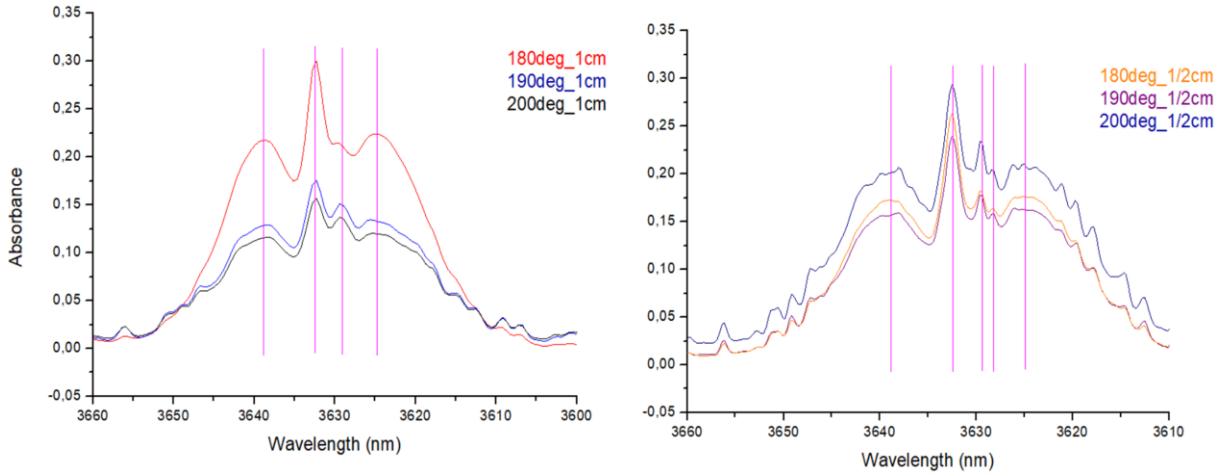


Figure 1. Gas infrared spectra of 2-fluorophenol.

Agradecimentos/Acknowledgments

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SAR studies on the chemical space expansion of a pyrazole hit.

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Palavras Chave:*Pyrazoles,SAR,Synthesis,Cytotoxicity,Hit-to-lead*

Highlights

Chemical space expansion of a pyrazole hit via electronic and steric modifications for SAR mapping against THP-1 leukemia cells.

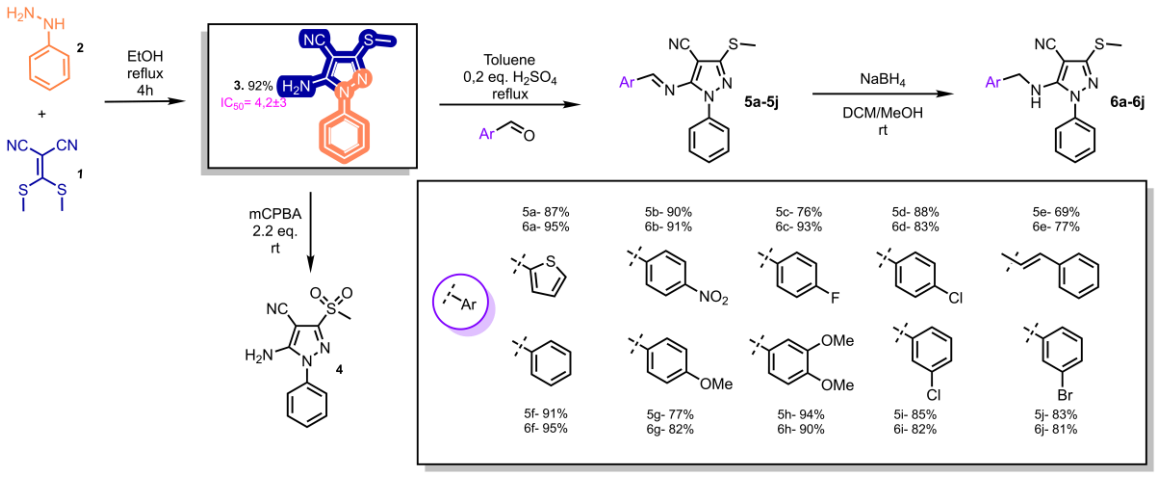
Resumo/Abstract

Pyrazole nucleus is a prominent scaffold in medicinal chemistry, recognized for its broad spectrum of biological activities[1]. Recently, our group identified a functionalized pyrazole hit (3) that exhibited promising cytotoxic activity against the THP-1 human monocytic leukemia cell line (IC_{50}=4.2±3 µM). Building upon this result, this work describes the expansion of the chemical space of this scaffold to explore structure-activity relationships through systematic modifications. The synthesis of the hit (3) was achieved via the cyclocondensation between an ethenodithioacetal (1) and phenylhydrazine (2) in ethanol under reflux, yielding the product in 92%. Starting from this intermediate, three diversification pathways were explored to modulate electronic and steric properties: selective oxidation of the sulfanyl group using mCPBA (2.2 eq.) to obtain the corresponding sulfone (4); the acid-catalyzed condensation with a series of 10 aromatic and heteroaromatic aldehydes, including derivatives with electron-withdrawing (NO_2, halogens), electron-donating (OMe), and heterocyclic (thiophene) groups, to form a library of imines (5a-j) with yields ranging from 69% to 94%; and the reduction of the imines using $NaBH_4$ to yield secondary amines (6a-j) with yields up to 95%. The structural modifications were designed to evaluate the impact of lipophilicity and electronic density, specifically probing the relevance of the hydrogen-bond donor site by its temporary removal in imines and subsequent restoration in secondary amines. All synthesized compounds were fully characterized by ^1H and ^{13}C NMR spectroscopy, confirming the structures. This strategic diversification of the hit's chemical space, covering a wide range of molecular volumes and electronegativities, is a fundamental step toward mapping the pharmacophoric requirements for optimizing cytotoxic activity against the THP-1 lineage[2].

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Synthesis and structural diversification of pyrazole 3 into derivatives 4, 5a-j, and 6a-j.

Agradecimentos/Acknowledgments

UFF

Selective Electrosynthetic Reduction and Diastereoselective Dimerization of Cinnamonitriles Using Solvent-Derived Protons

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Palavras Chave:*Electrosynthesis,Green chemistry,Reduction,Cinnamonitriles*

Highlights

Electrosynthesis enables selective reduction or diastereoselective dimerization of cinnamonitriles using solvent-derived protons, avoiding transition metals and pressurized H_2.

Resumo/Abstract

The reduction of carbon–carbon double bonds (C=C) is a cornerstone transformation in organic synthesis, traditionally achieved by catalytic hydrogenation using pressurized H_2 and noble metal catalysts. Despite its efficiency, this approach raises concerns related to safety, sustainability, and limited control over reaction pathways. In this context, electrosynthesis stands out as a sustainable and highly controllable alternative, employing electrons as clean reagents and enabling fine-tuning of reaction outcomes through precise control of the applied potential. Herein, we report a selective electrosynthetic methodology for the transformation of cinnamonitriles using solvent-derived protons (H_2O and/or methanol) as hydrogen sources, eliminating the need for molecular hydrogen. The reactions were conducted in an undivided cell with graphite electrodes, using DMSO/$LiClO_4$ as the reaction medium and supporting electrolyte under constant potential conditions. Remarkably, the methodology allows selective access to distinct reaction pathways: either the controlled reduction of the C=C bond or a competing electrodimerization process, the latter occurring with notable diastereoselectivity. Under optimized conditions, the reduced monomer was obtained in 60% isolated yield, while the diastereomerically enriched dimer was formed in up to 66% yield, with minimal formation of over-reduction byproducts (Figure 1). To evaluate the applicability of the method, a scope consisting of four cinnamonitrile derivatives was investigated. These results demonstrate that organic electrosynthesis constitutes a safe and sustainable alternative to conventional hydrogenation, eliminating the need for pressurized H_2 and noble metal catalysts, while simultaneously enabling precise control over chemoselectivity and stereochemical outcomes.

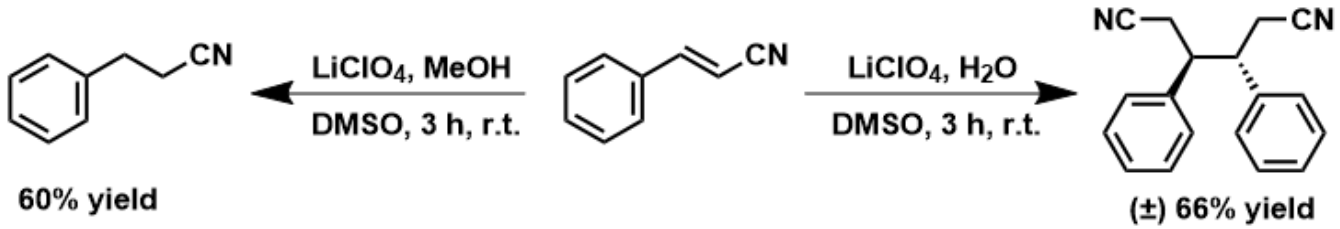


Figure 1 – Electrosynthetic reduction and diastereoselective dimerization of cinnamonitriles.

Agradecimentos/Acknowledgments

The authors are grateful for the financial support from CAPES, CNPq, UFJF, and FAPEMIG (APQ-01259-24).

Selective Synthesis of Pyridoxine-Derived Chalcones and 1,3,5-Triaryl-1,5-diketones via Controlled Aldol Condensation

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Palavras Chave:*Pyridoxine,Chalcones,Aldol condensation,Michael addition,Selectivity*

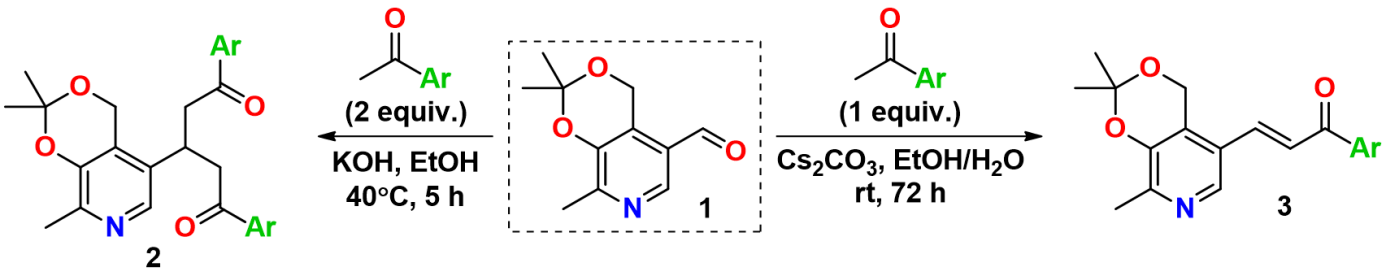
Highlights

Selective aldol conditions afford either chalcones or Michael adducts from pyridoxine-derived aldehydes.

Base, stoichiometry, and solvent control product selectivity.

Resumo/Abstract

Aldol-type condensations involving acetylpyridines or pyridinecarboxaldehydes are notoriously challenging when selective access to pyridyl chalcones is desired, as competitive formation of aldol and Michael-type addition products is commonly observed. Similar difficulties were encountered during our investigations on condensation reactions of pyridoxine-derived substrates, which contain a formyl-substituted pyridine ring, with methyl ketones. In this context, the present work aims to establish selective reaction conditions for the conversion of a pyridoxine-derived aldehyde into either chalcones or 1,3,5-triaryl-1,5-diketones. Pyridoxine was employed as the starting material and initially protected as a six-membered cyclic ketal in 61% yield using 2,2-dimethoxypropane in the presence of*p*-TsOH. Subsequent oxidation of the free hydroxymethyl group to the corresponding aldehyde was achieved in 68% yield using PDC. This aldehyde**1**was then subjected to Claisen–Schmidt condensation with acetophenone as a model reaction to optimize selectivity (**Figure**). Under conventional basic conditions, significant formation of a Michael addition product, resulting from the addition of a second equivalent of acetophenone to the initially formed chalcone, was observed. Optimization studies revealed that the use of excess KOH, 2 equiv. of acetophenone, and EtOH as solvent at 40 °C for 5 h favored the selective formation of the Michael adduct**2**. In contrast, the use of 1 equiv. of Cs_2CO_3, 1 equiv. of acetophenone, and an EtOH/H_2O (1:1) solvent system at rt for 72 h led to preferential chalcone**3**formation. Application of these optimized conditions to a range of aryl methyl ketones afforded 6 new 1,5-diketones**2**in 25–86% yield and 6 new chalcones**3**in 34–81% yield. All compounds were fully characterized by HRMS and ^{1}H and ^{13}C NMR spectroscopy. Overall, the proposed strategy enabled access to both product classes, although lower yields were observed for substrates bearing EWD groups.



Selective access to both 1,3,5-triaryl-1,5-diketones 2 and pyridoxyl chalcones 3.

Agradecimentos/Acknowledgments

This work was supported by UFGD, Fundect (124/2024), and Finep (MCTI/Finep/CT-Infra 01/2013 04.13.0448.00; MCTI/ Finep/CT-Infra-Proinfra 02/2014 04.18.0011.00). The authors thank CAPES for scholarships.

Síntese de derivados triazólicos da 8-aminolausona com potencial antineoplásico.

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Palavras Chave:*Naftoquinona,Câncer,Modificação estrutural*

Highlights

Amino group introduction into lawsone-based triazole derivatives and biological evaluation of the new compounds.

Resumo/Abstract

A classe das 1,4-naftoquinonas é vastamente explorada no campo medicinal em consequência à diversidade das atividades farmacológicas de seus derivados[1]. Entre eles, a lausona apresenta alto efeito citotóxico em linhagens de células cancerígenas[2],assim como as moléculas oriundas deste arcabouço molecular. Diante disso, recentemente foi evidenciado na literatura a atividade antineoplásica de derivados triazólicos**1.**Estes, por sua vez, apresentaram resultados positivos contra linhagem celular de melanoma (B16-F10) e adenocarcinoma pulmonar (A549)[3]. Deste modo, observando a escassez de estudos voltados à modificação estrutural do anel aromático do núcleo naftoquinona, o projeto tem como objetivo a síntese e análise de derivados triazólicos contendo o grupo amino nesta estrutura. A rota sintética realizada (Esquema 1) iniciou-se com a nitração da 1,4-naftoquinona**(1)**, que logo sofreu redução do grupo nitro, formando o grupamento amino, gerando**(3)**[4]**.**Em seguida, este intermediário obteve a morfolina adicionada em sua estrutura, por meio da reação de adição de Michael regiosseletiva, formando**(4)**, que posteriormente sofreu hidrólise, produzindo**(5)**. Sucedeu-se uma reação de propargilação, sintetizando**(6)**. Este intermediário, por sua vez, foi submetido à adição de azida aromática, gerando**(7).**No momento, os derivados da 8-aminolausona**(5)**estão sendo sintetizados variando o substituinte no anel aromático oriundo da azida.

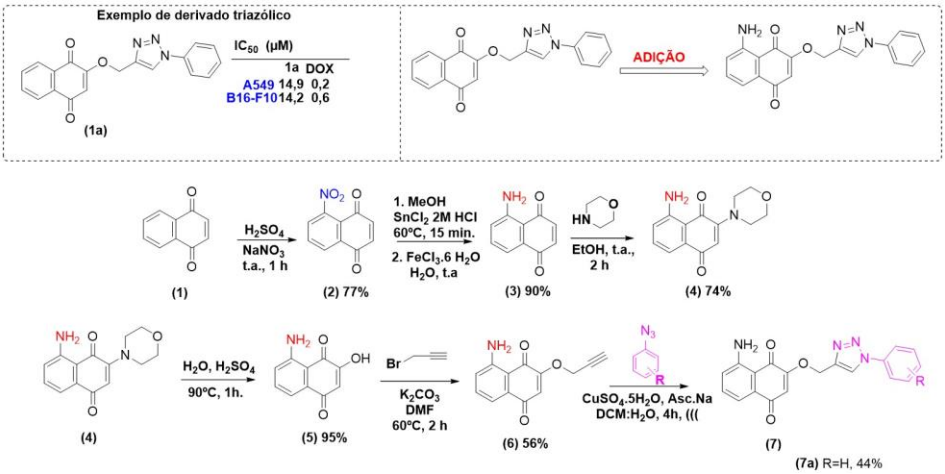
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Esquema 1. Rota sintética dos derivados triazólicos.

Agradecimentos/Acknowledgments

PPGQ-UFF, FAPERJ, CAPES, CNPQ e PIBIC.

Síntese de novos tioéteres e sulfonil-naftoquinonas derivadas da menadiona com potencial antitumoral

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Palavras Chave:*Vitamina K3, 2-metil-1,4-naftoquinona, tioéteres, sulfonas,2-metil-1,4-naftoquinona, tioéteres, sulfonas,Vitamina K3,2-metil-1,4-naftoquinona,tioéteres,sulfonas,câncer*

Highlights

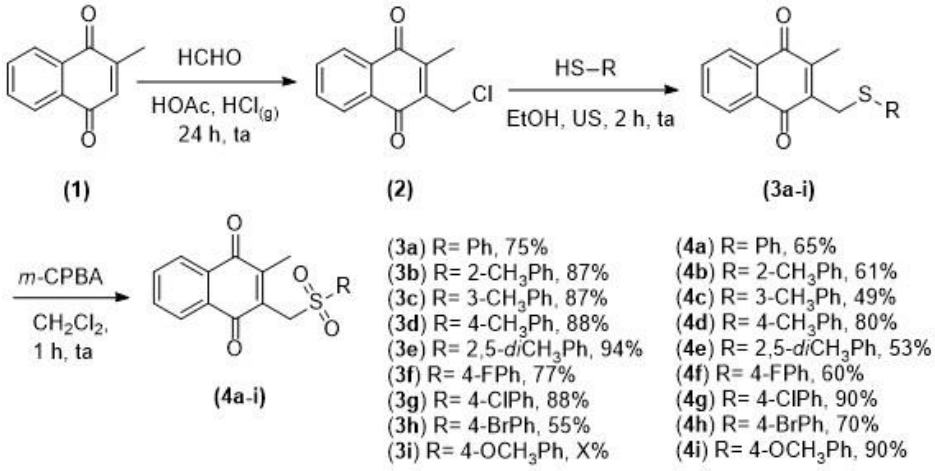
Synthesis of new menadione derivatives. Evaluation of the influence of the triazole moiety on the antitumor profile.

Resumo/Abstract

Câncer é um termo que se refere a um conjunto de doenças ligadas a mecanismos de crescimento e proliferação celular desordenados, representando um valor significativo das causas de morte no mundo, necessitando ainda hoje de novos tratamentos com maior seletividade e menos efeitos adversos.[1] As naftoquinonas são uma classe de substâncias amplamente descritas na literatura, devido seu diverso perfil biológico, podendo-se destacar a menadiona e seus derivados, que já foram relatados por possuírem perfil antitumoral, com ênfase para a combinação com o núcleo 1*H*-1,2,3-triazol, incentivando assim, nosso grupo de pesquisas no planejamento e síntese de novos híbridos funcionalizados com tioéteres e sulfonas contendo tal associação, os quais apresentaram atividade frente a diferentes linhagens de câncer de mama, em ensaios preliminares.[2,3] Nesse contexto, através da estratégia de simplificação molecular, este trabalho tem por objetivo a síntese de análogos destas substâncias com a ausência do núcleo triazólico com o intuito de avaliar a influência deste para a atividade antitumoral. Para isso, a rota sintética é apresentada no Esquema 1 e se inicia através da reação de clorometilação entre a menadiona**(1)**e*p*-formaldeído, sob fluxo de ácido clorídrico gasoso, obtendo-se o derivado**2**com 81 % de rendimento.[2] Este por sua vez é transformado em diferentes tioéteres**(3a-i)**por meio de uma substituição nucleofílica bimolecular empregando tióis comerciais. Por fim, uma oxidação dos tioéteres empregando*m*-CPBA levou a formação de nove sulfonas inéditas**(4a-i)**, com rendimentos entre 49-90%. Após o término da série todos tioéteres e sulfonas derivados da menadiona serão avaliados frente a diferentes linhagens tumorais.

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Esquema 1. Síntese dos tioéteres (3a-i) e sulfonas (4a-i) derivados da menadiona

Agradecimentos/Acknowledgments

Agradecimentos:PPGQ-UFF, FAPERJ, CAPES e CNPq

Síntese de Núcleos Benzoxazólicos no Âmbito da Química Verde utilizando Irradiação de Micro-ondas e Catálise Ácida

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Palavras Chave:*benzoxazóis,síntese,química verde,micro-ondas*

Highlights

Vanillin and benzaldehyde were successfully converted into bioactive benzoxazoles, green one-pot synthesis of benzoxazoles was achieved via microwave irradiation.

Resumo/Abstract

Os oxazóis são núcleos heterocíclicos aromáticos de grande relevância em fármacos e materiais funcionais, devido à sua versatilidade em ser sintetizado por múltiplas rotas. Conforme descrito por Quadros, Abenante e Lenardão (2022), trata-se de um anel aromático de cinco membros com oxigênio na posição 1 e nitrogênio na posição 3. Segundo Ramos (2024), o núcleo oxazólico é importante na química medicinal por apresentar diversas atividades biológicas, incluindo ações antibióticas, antivirais, antitumorais e antifúngicas. Nesse sentido, têm-se os derivados benzoxazóis, formados pela fusão do anel oxazólico a um anel benzênico, sendo muito utilizados em compostos bioquímicos e farmacêuticos e em diversas aplicações industriais, além de ser fundamental para uma extensa variedade de atividades biológicas (Bansal, 2021). Portanto, explorar novas estratégias de síntese que estejam alinhadas com os princípios da Química Verde é fundamental para avanços na síntese orgânica sustentável e para a obtenção destes produtos de interesse. Nesse contexto, destacam-se a síntese one-pot, as reações livres de solvente, o uso de catalisadores verdes e o uso da irradiação por micro-ondas. Assim, o presente trabalho realizou a síntese de benzoxazóis utilizando o-aminofenol como precursor sob irradiação de micro-ondas. Foram empregados dois aldeídos (vanilina e benzaldeído), avaliados tanto em condições livres de solvente (solvente-free) quanto em etanol (C_2H_5OH). A catálise ácida foi promovida por ácido cítrico (presente no suco de limão) e cloreto de zinco ($ZnCl_2$). As análises por espectroscopia de Ressonância Magnética Nuclear (RMN) confirmaram a formação do produto em todas as reações, demonstrando o êxito da metodologia proposta.

Agradecimentos/Acknowledgments

À FAPES pelo financiamento, à UFES pelo Programa de Pós-Graduação em Química e ao Laboratório Paulo Cezar Vieira.

Síntese de selonas N-heterocíclicas e suas diversas aplicações

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Palavras Chave:*selonas N-heterocíclicas,detecção de cádmio,Mayaro vírus*

Highlights

:Fluorescent selone was evaluated as a probe for Cd^{2+} detection. Trameric selone was active against*A.mayaro*. Dimeric selones were synthesized to obtain ruthenium complexes to be used in catalysis.

Resumo/Abstract

Nosso grupo tem utilizado 1-metilimidazol para a síntese de selonas*N*-heterocíclicas para diversas aplicações. Uma selona fluorescente foi sintetizada para servir como sonda na detecção de íons cádmio em raízes de*Typha domingensis*. Selonas mono-, di-, tri- e tetraméricas também foram obtidas para avaliação contra a infecção pelos arbovírus*Orthoflavivirus zikaense*(ZIKV),*Alphavirus chikungunya*(CHIKV),*Alphavirus mayaro*(MAYV) e*Orthobunyavirus oropoucheense*(OROV). Selonas diméricas estão sendo sintetizadas para a obtenção de complexos de rutênio que serão utilizados em reações catalíticas para a produção de H_2 a partir de borohidreto de sódio. Finalmente, estamos conduzindo um estudo sobre a influência de substituintes no*N*-3 de selonas*N*-heterocíclicas na atribuição inequívoca dos deslocamentos químicos de RMN em relação aos átomos de hidrogênio e carbono do anel imidazólico.

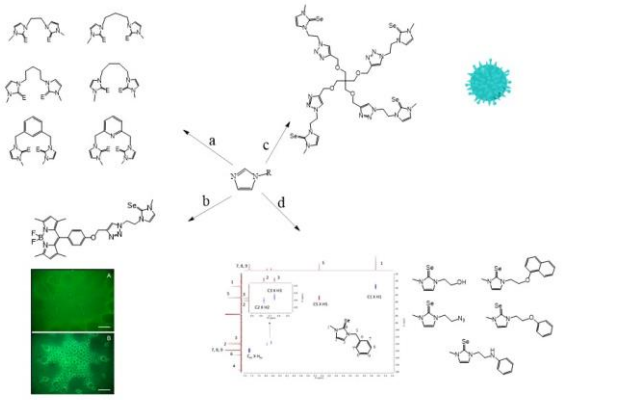


Figura 1 – Obtenção de derivados organocalcogênios descritos nesse trabalho. Em a) síntese de derivados diméricos de tionas, selonas e telonas N-heterocíclicas para testes de atividade biológicas e complexação com metais; b) selona fluorescente utilizada como sonda para detecção de íons cádmio em tecido vegetal; c) selona tetramérica com atividade para *Alphavirus mayaro*; d) selonas sintetizadas para estudo da influência de substituintes nos deslocamentos de sinais de ^{1}H e ^{13}C em RMN.

Selonas obtidas a partir do 1-metilimidazol e suas aplicações

Agradecimentos/Acknowledgments

Capes, FAPEMIG, PROPPI-UFOP, PPGQUIM-UFOP/ Laboratório Multiusuário de Caracterização de Macromoléculas do Programa de pós-graduação em Ciências Farmacêuticas CiPharma-UFOP.

Síntese e avaliação da atividade in vitro de derivados do hypofuran B e drynaram contra Trypanosoma cruzi.

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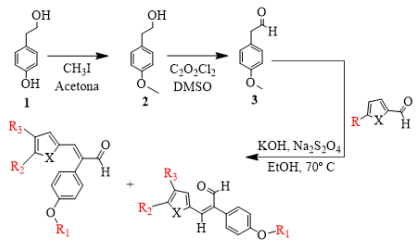
Palavras Chave:*furano,furfural,doença de chagas,antiparasitário,doenças negligenciadas*

Highlights

Hypofuran B and drynaran analogs were synthesized via crossed aldol condenstion and evaluated*in vitro*against*T. cruzi.*

Resumo/Abstract

A doença de Chagas é uma doença causada pelo protozoário*Trypanossoma cruzi*, cuja transmissão ocorre principalmente por picadas de inseto triatomíneos (barbeiros) e por ingestão de alimentos contaminados. Considerada pela OMS como uma doença negligenciada, a doença apresenta elevada prevalência em regiões pobres do planeta, principalmente na América Latina. No Brasil, a doença de Chagas ocorre principalmente na região Norte. O tratamento é dificultado pela baixa eficácia dos fármacos disponíveis na fase crônica e resistência variada das cepas do protozoário. No presente trabalho, os compostos naturais drynaran e hypofuran B e uma série de análogos foram sintetizados e testados in vitro contra*T. cruzi*. Para a síntese dos compostos, o tirosol foi submetido a oxidação de Swern e os aldeídos obtidos foram submetidos a reações de condensação aldólica cruzada com derivados do 5-hidroximetilfurfural. Os compostos foram obtidos em rendimentos entre 20% to 83% e razões diastereoisoméricas (E/Z) de 89:11 a 98:2. As atividades antiparasitárias foram avaliadas in vitro contra*T. cruzi*. Os compostos mais ativos (com baixos valores de IC_{50}) foram avaliados quanto à citotoxicidade em células L929 para determinação de CC_{50} e índices de seletividade ($IS=CC_{50}/IC_{50}$). O composto 22, apresentando anel tiofeno com grupo substituinte fenil na posição 5, foi o mais promissor, com baixo valor de IC50 (30,1 µmol L-1) apenas cerca de duas vezes maior que o do fármaco benzonidazol (IC50=14.1 µmol L-1). Entretanto, o composto apresentou elevada citotoxicidade e baixo valor de IS comparado ao fármaco usado como controle positivo. Os resultados servem como ponto de partida para a otimização da relação estrutura-atividade desta classe de compostos com o objetivo de se obterem moléculas promissoras para o desenvolvimento candidatos ao tratamento da doença de Chagas.



	X	R_1	R_2	R_3	(E/Z)
4	O	OH	CH_2OH	H	89:11
5	O	OCH_3	C_6H_5	H	88:12
6	O	OCH_3	4-NO_2-C_6H_5	H	92:8
7	O	OCH_3	4-Br-C_6H_5	H	88:12
8	O	OCH_3	4-Cl-C_6H_5	H	88:12
9	O	OCH_3	3-Cl-C_6H_5	H	93:7
10	O	OCH_3	2-Cl-C_6H_5	H	96:4
11	S	OCH_3	C_6H_5	H	96:4
12	S	OCH_3	H	C_6H_5	97:3
13	O	OCH_3	4,5-CH_3	H	94:6
14	O	OCH_3	CH_2CH_3	H	93:7
15	O	OCH_3	CH_3	H	96:4
16	O	H	CH_2OH	H	98:2
17	O	H	4-Br-C_6H_5	H	97:3
18	O	H	4-Cl-C_6H_5	H	87:13
19	O	H	3-Cl-C_6H_5	H	95:5
20	O	H	2-Cl-C_6H_5	H	100% E
21	S	H	C_6H_5	H	97:3
22	S	H	H	C_6H_5	98:2
23	O	H	4-NO_2-C_6H_5	H	96:4
24	O	H	4,5-CH_3	H	91:1
25	O	H	CH_2CH_3	H	90:10

Rota sintética e estruturas dos compostos derivados do hypofuran B e drynaran

Agradecimentos/Acknowledgments

Ao Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq – processo 401785/2023-8) e Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG – processo APQ APQ-01414-24) e à CAPES pelo suporte financeiro.

Síntese e caracterização de novos análogos triazólicos do fentanil

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Palavras Chave:*Fentanil,Anéis triazólicos,Reação click,Azida*

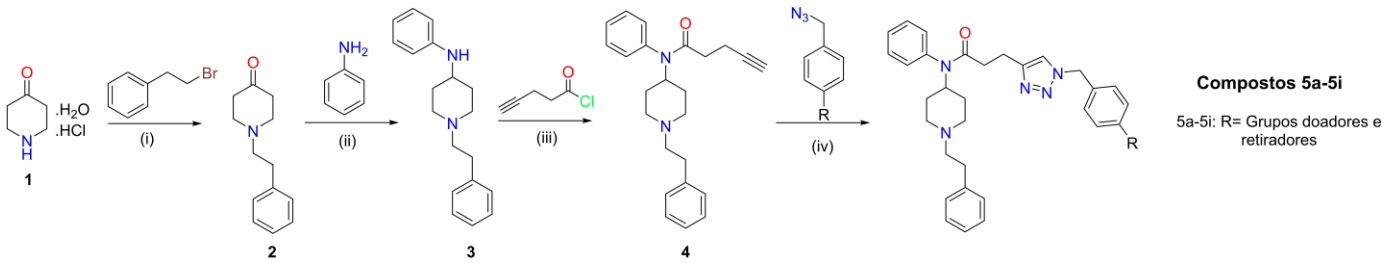
Highlights

Novel*N*-acyl triazole-containing fentanyl derivatives were obtained via click chemistry. All compounds and their intermediates were characterized by NMR, IR, and HRMS.

Resumo/Abstract

O fentanil é um opioide sintético altamente potente e de rápida ação analgésica, amplamente utilizado em ambiente hospitalar. Entretanto, seu uso pode levar a efeitos colaterais graves, como dependência química, depressão respiratória e constipação. Além disso, o crescimento dos casos do uso do fentanil como droga de abuso tem chamado a atenção em todo o mundo, resultando na recente e grave crise dos opioides. Embora centenas de derivados do fentanil tenham sido descritos nas últimas décadas, ainda há a necessidade da descoberta de análogos estruturais seguros, que mantenham a alta analgesia, porém com menos efeitos colaterais. A introdução de grupos heterocíclicos, tem se mostrado vantajosa na otimização de propriedades físico-químicas e afinidade por diferentes receptores alvo.[1]Neste contexto, este trabalho tem como objetivo sintetizar novos análogos 1,2,3-triazólicos do fentanil via reações de química “click”, para avaliação de seu potencial analgésicos. Na Figura está representada a rota sintética empregada para a obtenção dos análogos. A síntese inicia-se com a etapa de*N*-alquilação da piperidona (**1**), seguida pela aminação redutiva do composto**2**. Em seguida, para a introdução do alcino terminal, realizou-se a*N*-acilação da amina**3**e, posteriormente, realizou-se a reação de cicloadição do composto**4**com azidas benzílicas, levando à obtenção nove novos triazois fentanílicos do tipo**5 (5a-5i)**. As reações foram monitoradas por CCD e, quando necessário, os produtos foram purificados por cromatografia em coluna. Os novos derivados do fentanil obtidos e seus intermediários de síntese, foram caracterizados por meio de técnicas espectroscópicas e espectrométricas, como RMN, IV e HRMS. Como perspectiva futura, os análogos serão submetidos a estudos de interação com receptores relacionados a analgesia (MOR) e dependência (σ1R), com o objetivo de avaliar sua aplicação como novos candidatos terapêuticos.

1- Paulino, R. P. et al.*J. Braz. Chem. Soc.*2023, 69(5), 849.



Reagentes e condições: i) K_2CO_3, MeCN, 80ºC, 24h; 74%. ii) AcOH, $NaBH_4$, DCM, 40ºC, 24h; 68%. iii) DIPEA, DCM, 0ºC → t.a., 48h; 85%. iv) CuSO4, NaAsc., DCM/H_2O (1:1), t.a, 3h-5h; 67-98%.

Rota sintética dos intermediários 2–4 e da série de derivados do fentanil (5a–5i).

Agradecimentos/Acknowledgments

Este trabalho foi desenvolvido com o suporte financeiro da FAPEMIG e do CNPq.

Stoichiometry-controlled Chemoselective Mechanochemical Indolation of 1,2-Naphthoquinones Under Metal- and Solvent-free Conditions

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Palavras Chave:*Solvent-free,Metal-free,Indole,Naphthoquinone,Carbon-carbon*

Highlights

Mechanochemical indolation of 1,2-naphthoquinones Metal- and solvent-free synthesis of f novel hybrids Compounds with potential biological activity

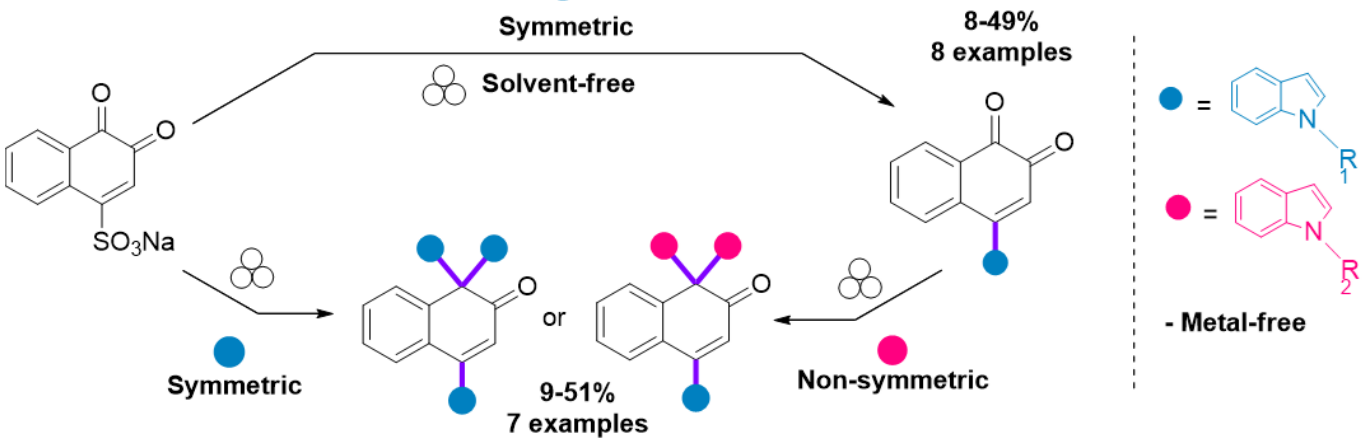
Resumo/Abstract

Indole-naphthoquinone derivatives represent a promising strategy for the development of new therapeutic agents, given the broad relevance of indoles and naphthoquinones in organic and medicinal chemistry.[1,2] The search for more effective and sustainable drugs has stimulated interest in hybrid structures that combine distinct bioactive scaffolds. The search for more effective and sustainable drugs has stimulated growing interest in hybrid structures that combine different bioactive scaffolds. However, the reported methods for the synthesis of 1,2-naphthoquinone derivatives often present significant limitations, including restricted substrate scope and poor environmental sustainability. In this work, the sodium salt of 1,2-naphthoquinone (β-NQSNa) was employed as a versatile reagent, either commercially available or readily prepared from β-naphthol. This reagent was used as a staring material with*N*-alkylated or free indoles to develop a methodology for the synthesis of conjugated 1,2-naphthoquinone derivates under catalyst-free conditions, which has recently been published by our group.[3] The reaction proceeds enabling carbon-carbon bond formation between the C3 position of the indole ring, bearing various N1 substituents, and the C4 position of the 1,2-naphthoquinone core, using bench-stable β-NQSNa as the reactant. This strategy affords 15 examples (8-51% yields) of mono- and trisubstituted derivatives, including both symmetric and non-symmetric products.

[1] Nguyen, H. Y.*et al*.*RSC Adv*.**2024**,*14*, 2341-2345;

[2] Dong, Y.*et al*.*ACS Omega*,**2019**,*4*, 21567-21577;

[3] Oliveira Lima Filho.*et al*.*Tetrahedron*.**2025**,*187*, 134917.



Synthesis of Mono- and Tris-indole 1,2-naphthoquinones.

Agradecimentos/Acknowledgments

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Studies on the Synthesis of furanchalcones

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[1]*Universidade Federal do ABC*

Palavras Chave:*Biomass,Furfural,Furanchalcones,Synthesis*

Highlights

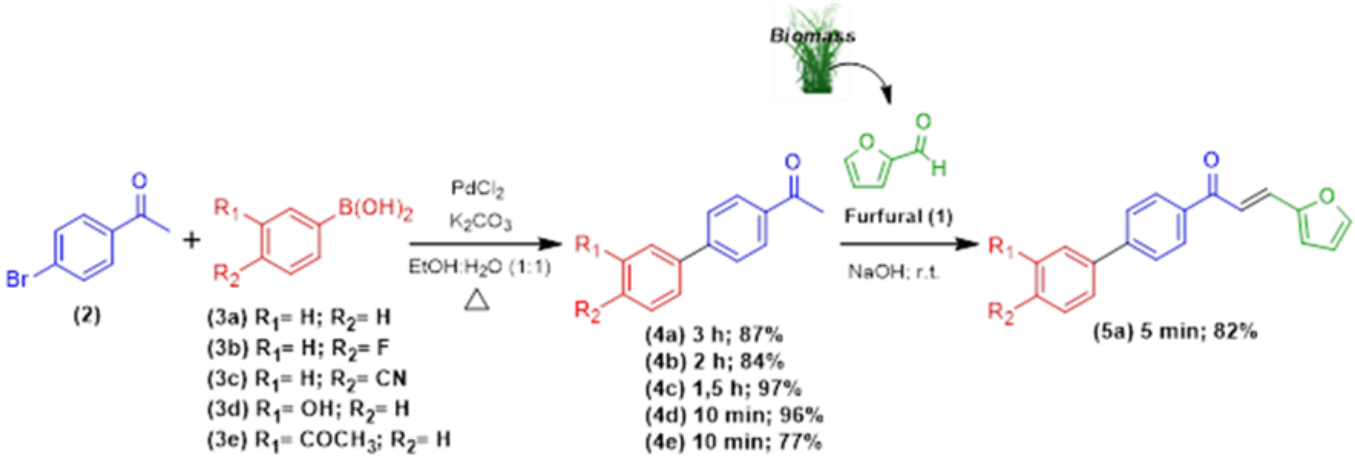
A new study on the synthesis of potentially bioactive furfural derivatives (furanochalcones) via Suzuki–Miyaura coupling and Claisen–Schmidt condensation.

Resumo/Abstract

Furfural (1) can be obtained from biomass hydrolysis (renewable source). It is a heterocyclic and aromatic aldehyde with a versatile structure, enabling a wide range of chemical transformations. Furanchalcones are hybrid-type molecules in medicinal chemistry, i.e., they contain two (or more) domains with distinct biological functions. In this work, a study was conducted on the synthesis of furanochalcones using furfural in one of the synthetic steps.[1] The synthetic route involved a Suzuki–Miyaura coupling followed by a Claisen–Schmidt condensation (Scheme 1).

Different procedures and reaction conditions were evaluated for the Suzuki–Miyaura cross-coupling of 4-bromoacetophenone (**2**) with phenylboronic acid (**3**). The optimal conditions involved reflux for 3 h, followed by catalyst removal by filtration through a silica gel column. Product**4a**was obtained in 87% yield and its structure was confirmed by NMR spectroscopy. The reaction was evaluated using substituted phenylboronic acids, resulting in different reaction times and product yields (77-97%). After obtaining compound**4a**, the Claisen–Schmidt condensation was optimized, affording furanochalcone 5a in 82% yield under solvent-free conditions. The results indicate that the studied methodology may be an efficient approach for the synthesis of furanochalcones.

[1] E. García,*et al.*Furanchalcone–biphenyl hybrids: synthesis, in silico studies, antitrypanosomal and cytotoxic activities.*Med. Chem. Res.***2019**,*28*, 608–622.



Synthesis of furanchalcones

Agradecimentos/Acknowledgments

To CAPES, for the scholarship, and to the Federal University of ABC

Studies Toward the Enantioselective Synthesis of the Miltochrista calamine Sex Pheromone (5R,7R)-5-Methylheptadecan-7-ol Using Chiral Auxiliaries

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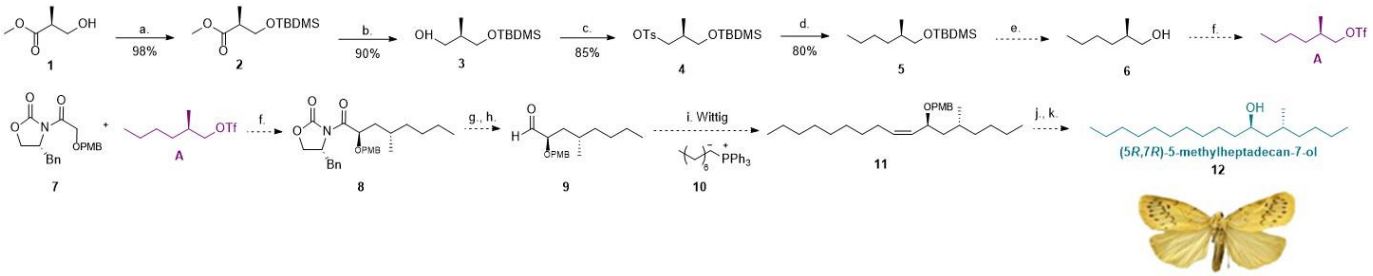
Palavras Chave:*Semiochemicals,Enantioselective synthesis,Chiral auxiliaries,Asymmetric synthesis*

Highlights

Development of an enantioselective synthetic route to the sexual pheromone of*Miltochristacalamina*,(moth), featuring stereochemical control of two chiral centers.

Resumo/Abstract

Insect pheromones are stereodependent semiochemicals that mediate mating and species recognition and are increasingly explored for environmentally benign pest management[1–3]. Because small stereochemical changes can elicit distinct behavioral responses[3], enantioselective syntheses are essential to supply well-defined material for bioassays and field trials. Here we describe progress toward a chiral-auxiliary-based route to the Miltochrista calamine sex pheromone, (5R,7R)-5-methylheptadecan-7-ol, identified in 2011[5] and first synthesized in 2014[6]. Our strategy couples fragment buildup with auxiliary-controlled stereochemical induction. A protected chiral alcohol fragment was prepared via TBDMS protection (a, 90% yield), reduction (b, 90%), tosylation (c, 85%), and chain elongation by nucleophilic substitution (d, 80%); further reduction and triflate formation are in progress. In the stereochemical phase, an L-phenylalanine-derived oxazolidinone auxiliary[4] bearing a bulky p-methoxybenzyl (PMB) group[7,8], will direct key C–C bond formation and enable auxiliary-directed 1,3-stereoinduction to install the C7 hydroxyl center. Final assembly is planned by Wittig coupling, followed by deprotection and hydrogenation to deliver the target enantioenriched alcohol for subsequent biological evaluation.
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Miltochrista calamina lutea (Staudinger, 1887)

Agradecimentos/Acknowledgments

The authors would like to thank CAPES, CNPq and INCT - BioInnovations for sustainable agriculture for funding.

Study of Spirocyclopropanation in Erlenmeyer-Plöchl Azlactones Using Sulfoxonium Ylides

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Palavras Chave:*Azlactones,Spirocyclopropanation,Michael-type,Concerted,Ylides*

Highlights

A spirocyclopropanation protocol was optimized for azlactone and sulfoxonium ylides, and DFT studies were carried out to propose a reaction mechanism for this transformation.

Resumo/Abstract

The Erlenmeyer-Plöchl azlactone is a scaffold widely used in the synthesis of various non-natural amino acids, which serve as key building blocks for the development of new bioactive compounds, both natural or synthetic. Consequently, modifications to this framework have been extensively explored through new synthetic methodologies, along with a deeper understanding of the mechanisms governing these transformations to improve the synthesis of new compounds.[1]

Reactions involving sulfur ylides, which act as carbanion sources commonly employed as alternatives to diazo compounds in organic chemistry,[2] can lead to the formation of azlactones bearing a three-membered ring via spirocyclopropanation. Although the formation of this product using sulfonium ylides has been reported, no studies have described the corresponding reaction mechanism, nor have there been reports of obtaining the same product from sulfoxonium ylides.[3]

In this work, the spirocyclopropanation product resulting from the reaction between the Erlenmeyer-Plöchl azlactone and a sulfoxonium ylide was obtained in 90% yield with a diastereomeric ratio of 3:1, and the reaction conditions were optimized (Figure 1). After structural elucidation of the major diastereomer by X-ray diffraction, the concerted addition and Michael-type addition mechanisms were investigated using Density Functional Theory (DFT). For each mechanism, hybrid GGA and hybrid meta-GGA functionals were employed, respectively, using the def2-SVP basis set.[4] Preliminary results indicate that the concerted addition pathway is the most promising.

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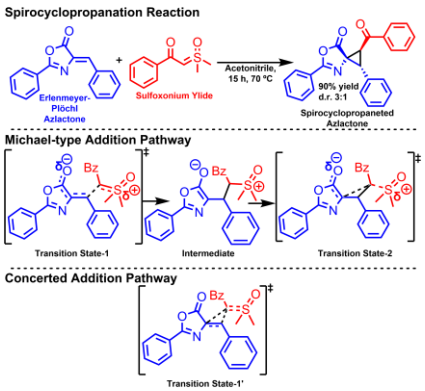


Figure 1. Spirocyclopropanation with the proposed reaction mechanisms.

Agradecimentos/Acknowledgments

The authors are grateful for the generous financial support from CAPES (Finance Code 001), CNPq, UFJF, and FAPEMIG.

Sulfur-Based Systems in Modern Organic Synthesis: Selective Control of Alkyne Reactivity

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Palavras Chave:*stereoselective reduction,chemodivergent synthesis,alkynes*

Highlights

Sulfur nucleophiles enable regioselective alkyne transformations, affording (E)-alkenes and sulfur-rich heterocycles via reduction, cyclization, and ring contraction.

Resumo/Abstract

The addition of nucleophilic sulfur species to C≡C bonds is a valuable strategy for the construction of organic molecules with potential technological and pharmaceutical relevance. In this lecture, we will explore this synthetic approach in sulfur-based systems, focusing on the regioselective addition of sulfur nucleophiles to molecular structures containing C≡C bonds, with the aim of accessing relevant products through cyclization and reduction reactions.

We will present our results on the use of the trithiocarbonate anion (CS_3^{2-}), generated in situ from the CS_2/KOH system, as a low-cost synthetic equivalent for the stereoselective reduction of internal alkynes to afford*(E)*-alkenes. In addition, we will discuss a chemodivergent methodology for the synthesis of 1,4-benzo[*b*]dithiins and 1,4-benzodithiafulvenes through the addition of NaSH to 2-iodoaryl thioalkynes, followed by solvent-controlled cyclization or ring contraction reactions (Figure 1).

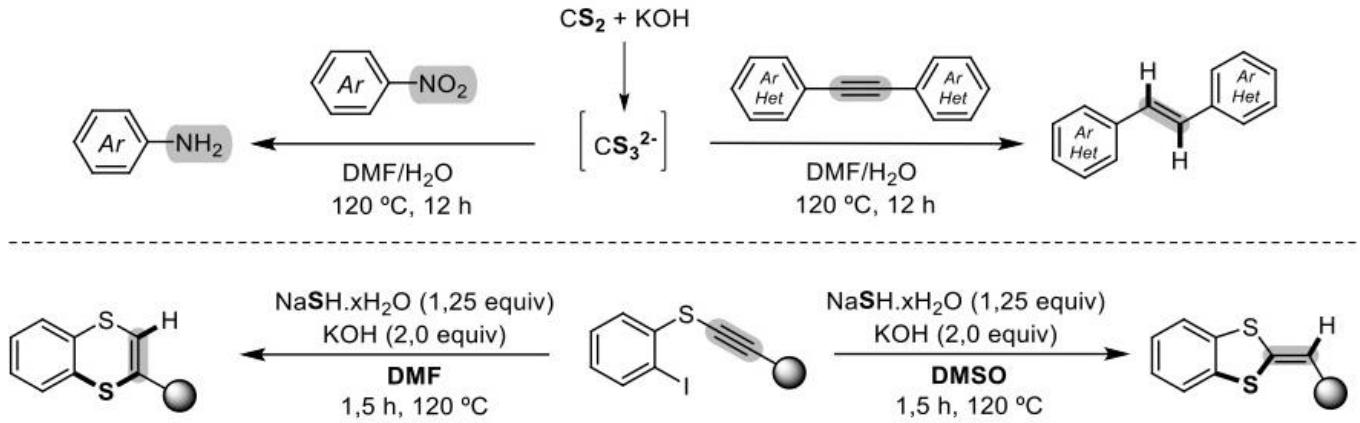


Figure 1

Agradecimentos/Acknowledgments

We are grateful to Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001, CNPq, (404503/2021-7, 308487/2021-4), FAPERGS (RITEs-RS and 24/2551-0001308-3)

Sustainable Electric-Field-Assisted Catalyst-Free Synthesis of Ethyl Biodiesel

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Palavras Chave:*Electrolysis,Catalyst-free synthesis,Ethyl biodiesel,Vegetable oils,Sustainable biofuels*

Highlights

- Electric-field-assisted, catalyst-free ethyl biodiesel synthesis.
- High yields from vegetable oils using ethanol.
- Sustainable and scalable electrochemical route.

Resumo/Abstract

This study investigates the electrolytic synthesis of ethyl biodiesel without conventional chemical catalysts, using a constant-voltage power source to evaluate reaction conditions and the performance of different vegetable oils. Emphasis is placed on renewable feedstocks, sustainability, and process simplicity [1]. A dedicated equipment was designed for this purpose, featuring a custom electrolytic power supply based on an LM338 integrated circuit and a parallel resistor bank (8.2–100 Ω), allowing precise control of the applied current. Two graphite rod electrodes (10 mm diameter) were positioned 10 mm apart. Experiments were carried out with different vegetable oils to assess the efficiency and robustness of the system. Ethanol (95%) was used at a 1:9 oil-to-alcohol volumetric ratio, and sodium chloride was added as a supporting electrolyte at 3% m/m relative to the oil. During electrolysis, all oils exhibited a characteristic electrical behavior. Under an initially quasi-constant current (~123 mA), the applied voltage gradually increased, indicating a progressive rise in the electrical resistance of the reaction medium (Figure 1). This behavior is attributed to physicochemical changes during transesterification, including phase evolution, depletion of ionic species, and changes in dielectric properties. At the final stage, a marked decrease in current accompanied by a sharp voltage increase was observed, suggesting the formation of a more resistive medium as biodiesel production advanced. Despite minor variations among the oils, similar electrical trends were observed across all systems, demonstrating the stability and reproducibility of the developed equipment. The process achieved biodiesel yields above 90% without chemical catalysts. Future work will focus on process optimization, scale-up, fuel characterization, and mechanistic studies. [1] Clean Energy, 2021, 19–31.

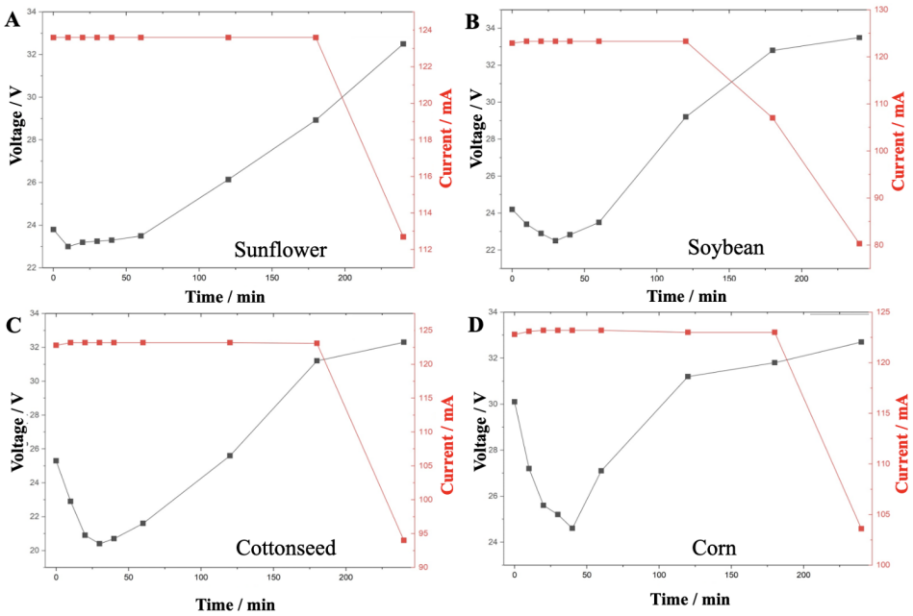


Figure 1. Voltage and current profiles recorded during the electrolytic synthesis of ethyl biodiesel

Agradecimentos/Acknowledgments

FAPEMIG, Capes, CNPQ

Synthesis and characterization of benzimidazolone derivatives with potential biological activities

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Palavras Chave:*Potencial biological activity; Isoxazole; Triazole; Organic synthesis*

Highlights

Development of new molecular hybrids with biologically relevant heterocycles linked to a benzimidazolone scaffold, still unexplored.

Resumo/Abstract

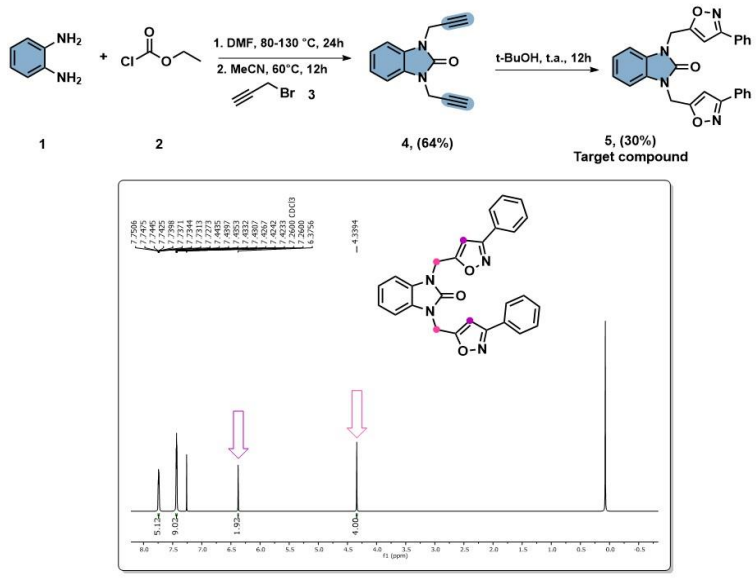
Benzimidazolone is a heterocyclic core of considerable relevance in medicinal chemistry, with chemical versatility and ability to interact with multiple biological targets, being associated with pharmacologically relevant activities such as anticancer, antiviral, and neuroprotective effects.[1] In this context, the hybridization of this scaffold with well-established bioactive heterocycles, such as isoxazole and triazole, represents a promising strategy for modulating and potentially enhancing biological profiles[2],[3] In view of this, the development of new chemical entities combining these heterocyclic frameworks is highly relevant. Herein, we report the synthesis of benzimidazolone and its subsequent functionalization with heterocyclic moieties. In the first step, phenylenediamine (1) was reacted with ethyl chloroformate (2), affording the corresponding benzimidazolone in 74% yield. This intermediate was then subjected to propargylation using propargyl bromide (3), leading to the propargylated benzimidazolone derivative (4) in 64% yield. This approach provides a versatile platform for structural diversification through further functionalization, including selenium-based transformations, 1,3-dipolar cycloaddition reactions for the synthesis of 1,2,3-triazoles, and cross-coupling reactions. As an initial proof of concept, the methodology was applied to the synthesis of an isoxazole-containing derivative, according to a synthetic methodology adapted from the literature[4], which was obtained in 30% yield. Current efforts are focused on optimizing the reaction conditions to improve yields and enable further expansion of the reaction scope.

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Reaction scheme and RMN of the target compound

Agradecimentos/Acknowledgments

UFF, CNPq, CAPES, FAPERJ.

Synthesis and characterization of novel phosphoramidate-linked 4-quinolone-3-carboxamides as potential antitumoral agents

Fernanda da Costa Santos Boechat (PQ)*[1], Rodrigo Luis Moreira Gomes (PG)[1], Lívia Maria Mendonça Augusto (PG)[1], Maria Cecília Bastos Vieira de Souza (PQ)[1], Istefani Luciene Dayse da Silva (PQ)[1].

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Palavras Chave:*Quinolone, antitumoral, phosphoramidates, 4-quinolone-3-carboxamides*

Highlights

A novel series of phosphoramidate-linked 4-quinolone-3-carboxamides was synthesized in moderate to high yields (33–89%) and is under in vitro evaluation against A375 and SK-MEL melanoma cells.

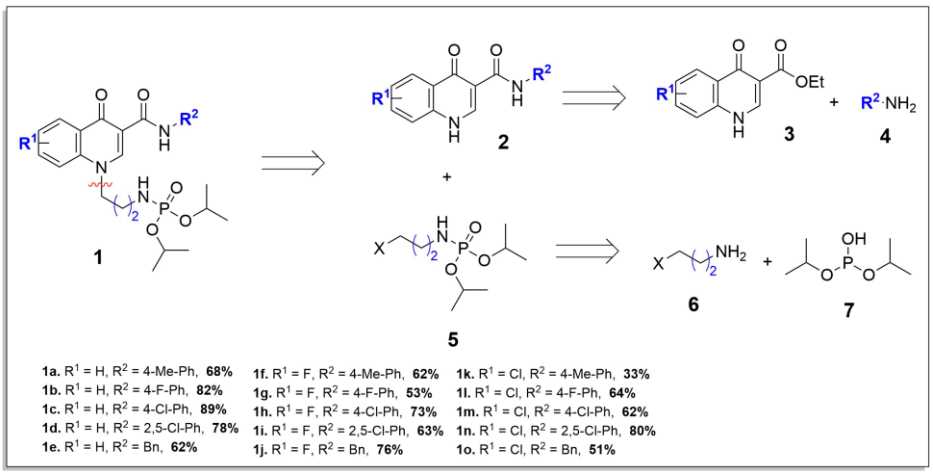
Resumo/Abstract

The synthetically versatile 4-quinolone scaffold is described in the literature as a privileged structure in medicinal chemistry, with a broad range of biological applications. Beyond their classical antimicrobial potential, derivatives of this class act as antifungals, antiparasitics, anxiolytics, antitumors, and antivirals. In particular, 4-quinolones containing a carboxamide moiety on the C-3 position (4-quinolone-3-carboxamides) stand out as promising drug candidates, as described in previous works by our research group, which focused on derivatization and hybridization strategies aimed at optimizing and tuning the biological activity of these derivatives. In light of this potential, this project proposes the synthesis and characterization of a novel series of 4-quinolone-3-carboxamides. Multiple derivatizations have been explored, including halogenation at strategic positions and the coupling of phosphoramidates to the nitrogen atom of the quinolone core, connected through methylene chains. These modifications seek to establish structure-activity relationships (SAR) and to generate molecules capable of overcoming limitations such as toxicity, low bioavailability, and resistance. To date, 15 derivatives have been obtained with yields ranging from 33% to 89% via the reaction of 4-quinolone-3-carboxamides with diisopropyl N-(3-chloropropyl) phosphoramidate under optimized conditions. In addition, some precursor 4-quinolone-3-carboxamides not previously reported in the literature were obtained. The 15 phosphoramidate-containing derivatives, along with their 15 precursor carboxamides, are currently in the initial phase of*in vitro*testing against the A375 and SK-MEL melanoma cell lines.

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Dine, I.; Mulugeta, E.; Melaku, Y.; Belete, M.*RSC Advances*, vol. 13, p. 8657-8682,**2023**.

Forezi, L.S.M.; Ribeiro, M.M.J.;et al*Eur. J. Med. Chem.*194, 112255,**2020**



Scheme 1. Synthetic planning and reaction yields for the methylene-bridged phosphoramidate

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES (Finance Code 0001)

Synthesis and corrosion inhibition evaluation of oxazolidines from ketene dithioacetals

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Palavras Chave:*synthesis,heterocyclic,ketenedithioacetals,oxazolidines,corrosion inhibitors*

Highlights

Synthesis of oxazolidines derivatives using ketenedithioacetals and their evaluation as corrosion inhibition.

Resumo/Abstract

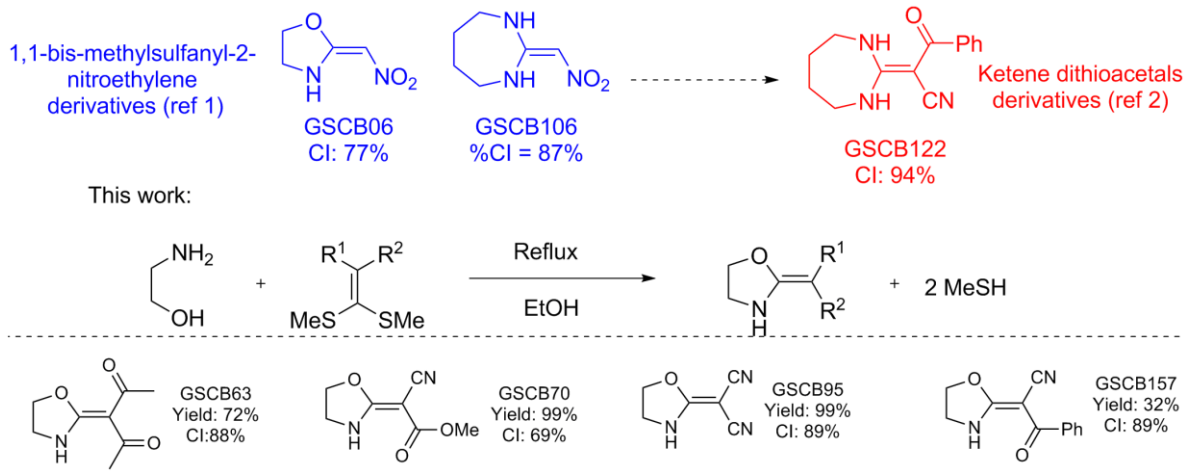
Steel structures can suffer damages like corrosion, an oxidation process by the environment. This issue has economic consequences and for that it starts a race for better corrosion inhibition and environmentally friendly compounds, specially the organic one who has more biodegrability.[1],[2]

Ketene dithioacetals are a very versatile building block, they can undergo to double vinlic substitution to produce heterocyclic scaffolds. Recently, we used 1,1-bis-(methylsulfanyl)-2-nitroethylene to produce different 2-nitromethylene heterocycles to investigate their efficiency as corrosion inhibition. When 2-nitromethylene diazepane (GSCB106) presented the most corrosion inhibition efficiency. After that, we also investigated diazepine derivatives varying other substituents in the position 2.[3]

In this work, using ethanolamine as a nucleophile we performed double vinylic substituition in ketene dithioacetals to produced four oxazolidine derivatives with an high and moderate yield and evaluate their corrosion inhibition.[4] Mass loss tests were performed for the produced compounds. Pieces of steel carbon SAE 1020 were submitted to a corrosive environment containing 1 M HCl solution with and without the synthetized oxazolidines. After a period of 4 hours in conditions to perform the oxidation of metal pieces were observed that changing the substitution group changes the efficiency of the corrosion inhibition. The compounds GSCB 95 and GSCB 157 were the most efficient.

In conclusion, combination of satisfactory synthetic yields(32-99%) and effective corrosion inhibition highlights the potential of oxazolidine derivatives as promising organic corrosion inhibitors.

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4 Sangi D, P. et al. Journal of the Brazilian Chemical Society, 25, 887-889, 2014



Synthesis of oxazolidines derivatives from ketenedithioacetals

Agradecimentos/Acknowledgments

UFF

Synthesis and Electrochemical Evaluation of Novel Coumarin-Based Diacylhydrazides

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Palavras Chave:*Coumarin,Composite materials,Heterocycles,Eletrochemical sensors*

Highlights

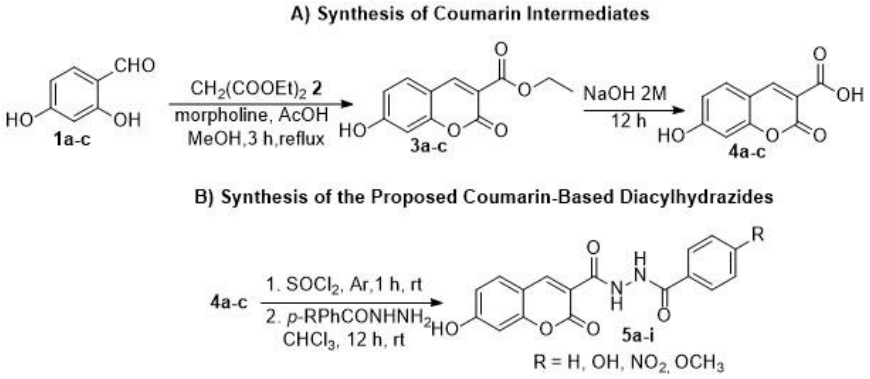
Synthesis of coumarin derivatives and their use in electrode modification to evaluate electrochemical performance, investigating the influence of different substituents by cyclic voltammetry

Resumo/Abstract

Electrochemical sensors are widely used in various fields of interest, which has driven the development of strategies aimed at improving their analytical performance. The modification of electrochemical interfaces with organic materials has proven to be an effective approach to enhance the sensitivity and selectivity of these sensors. Among the classes of organic compounds explored for electrochemical interface modification, coumarins are well known for their versatile chemical and biological properties, which have inspired research into their application in functional materials. Diacylhydrazides, owing to their strong coordination ability and thermal stability, have also shown great potential in the development of composite materials. The combination of coumarin and diacylhydrazide moieties may therefore lead to novel composite materials with enhanced electrochemical properties. The present work aims at the development of new coumarin-based diacylhydrazides, the fabrication of modified electrodes, and the evaluation of these composite materials as surface modifiers for electrodes. For the synthesis of**5**, a Knoevenagel condensation between 2,4-dihydroxybenzaldehyde (**1**) and diethyl malonate (**2**) was performed, affording**3**in yields ranging from 60% to 83%. The coumarins**3**were subjected to basic hydrolysis to obtain the corresponding acids**4**, which were subsequently reacted with thionyl chloride under an inert argon atmosphere to form the corresponding acid chlorides. These intermediates were then converted into**5**through nucleophilic substitution reactions with 4-substituted benzhydrazides, yielding products in the range of 85% to 93% (Scheme 1). The structures of all synthesized compounds were confirmed by physical characterization methods, and their behavior as electrochemical modifiers, applied via drop-casting technique, was evaluated using cyclic voltammetry.

BARANWAL, J.*et al, Chemosensors,**2022**, 10, 363*

MANJUNATHA, B.*et al, RSC Sustainability,***2023**, 2, 475



Scheme 1. Synthesis of coumarin-based diacylhydrazides 5.

Agradecimentos/Acknowledgments

FAPERJ, CAPES and CNPq

Synthesis and Study of Novel Functional N,N-Ligands for the Enantioselective Heck-Matsuda Reaction

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Palavras Chave:*Heck-Matsuda,Assymetric Catalysis,Ligands,Enantioselectivity*

Highlights

Novel PyrOx ligands applied in Heck-Matsuda reaction. Electron-withdrawing groups enhanced enantioselectivity. Yields up to 99% and 90% ee.

Resumo/Abstract

Asymmetric catalysis is one of the pillars of organic chemistry, as it enables the construction of complex molecules with high enantioselectivity. In this context, the enantioselective Heck-Matsuda (HM) reaction—a palladium-catalyzed C–C coupling between olefins and arenediazonium salts—stands out as a powerful tool for the synthesis of diverse classes of molecules. Thus, the success of asymmetric catalysis intrinsically depends on the chiral ligand, as its coordination to palladium induces the formation of the preferred enantiomer. Therefore, N,N-bidentate ligands are widely employed in the literature and in our research group due to their efficiency in pre-catalyst formation and stabilization of the metal center.

This work describes the development of novel Pyrazine-Oxazoline (PyrOx) ligands for application in HM reactions, aiming to open new synthetic routes for value-added products. The ligands were synthesized in three steps from 5-substituted pyrazinoic acids, involving esterification, amide formation with (L)-tert-leucinol, and cyclization with DAST. Ligands containing electron-withdrawing and electron-donating groups (CF_3, Cl, OMe, H) on the pyrazine ring were obtained.

In the catalytic evaluation (desymmetrization reaction of dimethyl cyclopent-3-ene-1,1-dicarboxylate with $Pd(TFA)_2$ in MeOH at 40°C), it was observed that electron-withdrawing groups favored selectivity. Ligand L1 (CF_3PyrOx) showed the best initial performance in terms of enantioselectivity (87:13 e.r.). This trend was rationalized through Linear Free Energy Relationship (LFER) analyses, confirming the electronic influence on the enantioselectivity-determining step. Finally, optimization of conditions and variation of diazonium salts resulted in excellent yields ranging from 84% to 99% and enantiomeric excesses (ee) between 76% and 90%, consolidating the potential of the PyrOx class as ligands for the enantioselective Heck-Matsuda reaction.

Synthesis, Molecular Docking and Anticancer Evaluation of Thiazolopyrimidines Targeting Kinesin Eg5

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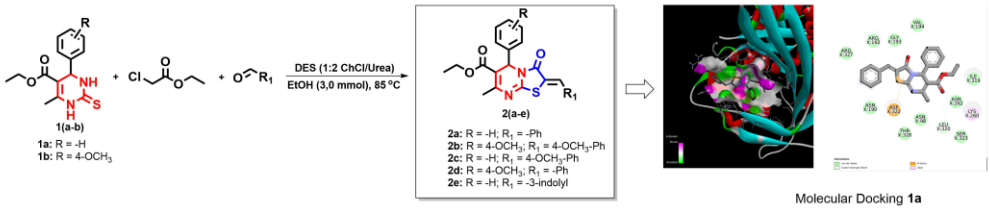
Palavras Chave:*Thiazolopyrimidines,Biginelli reaction,Kinesin Eg5,Deep eutectic solvents,Molecular docking*

Highlights

Green synthesis of thiazolopyrimidines from Biginelli scaffolds. Non-classical allosteric binding to kinesin Eg5 revealed by docking. Enhanced selectivity against cancer cells versus DHPMT precursors.

Resumo/Abstract

Thiazolopyrimidines are fused bicyclic heterocyclic compounds formed by a thiazolidinone ring, a five-membered heterocycle containing S, N, and a carbonyl group, fused to a six-membered pyrimidine ring containing two nitrogen atoms. These compounds are obtained from Biginelli reaction products, such as dihydropyrimidinethiones (DHPMTs), through cyclocondensation reactions with haloacids or their esters, generally using acetic acid as a catalyst and sodium acetate melted in acetic anhydride. However, DHPMTs, the synthetic precursors of these structures, primarily target kinesin Eg5, a motor protein essential for the mitotic process. In this context, it becomes relevant to investigate whether the structural conversion of DHPMTs into thiazolopyrimidines is able to preserve or enhance inhibitory activity against Eg5. In this work, five thiazolopyrimidines were synthesized through a multicomponent reaction involving DHPMTs, ethyl chloroacetate, and aromatic aldehydes, using a deep eutectic solvent composed of choline chloride and urea as the reaction medium. The compounds were obtained in yields ranging from 27–81% and were characterized by melting point determination, infrared spectroscopy, and ^{1}H and ^{13}C NMR spectroscopy. Molecular docking studies against the Eg5 protein (PDB: 1X88) indicated that thiazolopyrimidines interact with a non-conventional allosteric site, distinct from the classical loop-5 binding site. The inhibitory potential against the Eg5 molecular target was indirectly evaluated through cytotoxicity assays in tumor cell lines (HCT 116, MCF-7, HepG2, and AGS) and the non-tumor cell line L929, revealing a superior selectivity profile compared with DHPMTs, possibly associated with interaction with this alternative allosteric site.



Molecular Docking **1a**

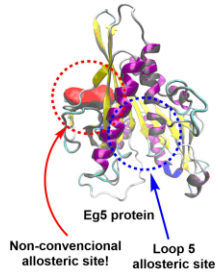


Table - IC50 values of the samples in tumor cell lines.

Samples	HCT 116 IC50 µM	Selectivity (IC50 L2929/IC50 HCT-116)	MCF-7 IC50 µM	Selectivity (IC50 L2929/IC50 MCF-7)	Hep-G2 IC50 µM	Selectivity (IC50 L2929/IC50 Hep-G2)	AGS IC50 µM	Selectivity (IC50 L2929/IC50 AGS)	L929 IC50 µM
1a	58.78 ± 1.6	0.434± 0.02	30.78 ± 1.5	**0.83± 0.06**	32.67 ± 1.4	**0.78± 0.05**	20.54 ± 1.2	**1.24± 0.10**	25.5 ±1.3
1b	50.61± 1.6	0.334± 0.02	77.3 ± 1.9	0.219± 0.02	21.1 ± 1.2	**0.80± 0.07**	6.05 ±0.7	**2.79± 0.38**	16.9 ±1.2
2a	49.55 ± 1.5	6.41± 0.2	53.06 ± 1.4	**5.99± 0.17**	143.6 ± 2.0	**2.21± 0.03**	181.8 ± 0.7	**1.75± 0.01**	317.8 ± 2.3
2b	>800	< 0.342	58.32 ± 1.6	**4.70± 0.13**	69.23 ±1.7	**3.96± 0.10**	119.6 ± 1.7	**2.29± 0.04**	273.9 ± 2.1
2c	54.84 ±1.5	7.96± 0.22	>800	< 0.546	69.21 ±1.7	**6.31± 0.16**	75.38 ± 0.3	**5.79± 0.04**	436.6 ± 2.5
2d	29.68 ± 1.2	**15.75± 0.64**	79.4 ± 1.9	**5.89± 0.15**	348.1 ± 2.3	**1.34± 0.01**	>800	> 0.58	467.4 ± 2.4
2e	43.09 ± 1.3	9.58± 0.30	57.26 ±1.6	**7.21± 0.21**	59.39 ± 1.6	**6.95± 0.19**	64.61 ± 1.9	**6.39± 0.19**	412.8 ± 2.6
Monastrol	58.33 ± 1.6	5.26± 0.15	49.08 ± 1.5	**6.25± 0.20**	86.50 ± 1.6	**3.55± 0.07**	323.5 ± 0.9	**0.95± 0.01**	306.7 ± 2.4
Cisplatin	-	-	52.85 ± 4.8	0.46 ± 0.13	54.68 ± 0.08	0.44± 0.11	39.59 ± 0.66	0.61± 0.15	24.05 ± 6.04
5-fluorouracil	37.00 ± 18.22	**13.0± 6.5**	-	-	-	-	-	-	481.83 ± 43.33

Legend: red = more cytotoxic than the control; blue = less cytotoxic than the control to the non-tumoral cell line; **bold** = better SI than the control.

Synthesis, docking, biological assays and unconventional allosteric site of 2(a-e).

Agradecimentos/Acknowledgments

The authors acknowledge CNPq, CAPES, FAPES, LabPetro (Center of Competence in Petroleum Chemistry), and the Federal University of Espírito Santo (UFES) for financial and institutional support.

Synthesis of 1,3-bis(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)propan-2-one: A possible bistriazole as a multidentate ligand in coordination compounds

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Palavras Chave:*Click chemistry,CuAAC,Organic Synthesis*

Highlights

Synthesis of 1,4-disubstituted 1,2,3-triazoles via*CuAAC*reaction. Study of chelating capacity and geometry of complexes. Synthesis and evaluation of Cu(II)-triazoles as neuroprotective agentes.

Resumo/Abstract

Triazoles compounds can be obtained via the*CuAAC*reaction, in which 1,4-disubstituted 1,2,3-triazoles are formed as the regioselective products. Some of these compounds are isolated as copper complexes and are purified using an EDTA-saturated solution, a common chelating agent. However, when an organic solution of derived bistriazole from propargyl alcohol**1a**was mixed with EDTA, the triazole migrated to the aqueous phase, resulting in a complex mixture. Several analyses were performed to characterize the coordination compound obtained. XRF analysis indicated that the crude product contained 96.42% copper and the UV–Vis spectrum showed a maximum absorption at 218 nm and an additional band at 210 nm,[1] corresponding to the Cu^{2+} ion absorption region. The TGA/DTG curves revealed mass loss due to water release above 100 °C (A), probable melting of the compound at 220 °C**(B)**, and thermal decomposition at 350 °C**(C)**. The residual mass stabilized at 0.4361 mg, attributed to the formation of CuO. Previous studies have demonstrated that triazoles can act as multidentate ligands in metal complexes, and that amine-based copper complexes exhibit activity against Alzheimer's disease. Therefore, the investigation of compound**1a**and its chelating capacity is of significant interest.[2,3,4] To obtain copper-free**1a**via an alternative route, bistriazole**1b**was synthesized and purified using an ethyl acetate/EDTA mixture. A carbonyl protecting group was introduced to afford compound**5**, which was reduced with $LiAlH_4$ under an inert atmosphere and subsequently deprotected by acidic hydrolysis to**1a**. Consequently, coordination compounds employing triazole**1a**as a ligand and their biological activity can be investigated.

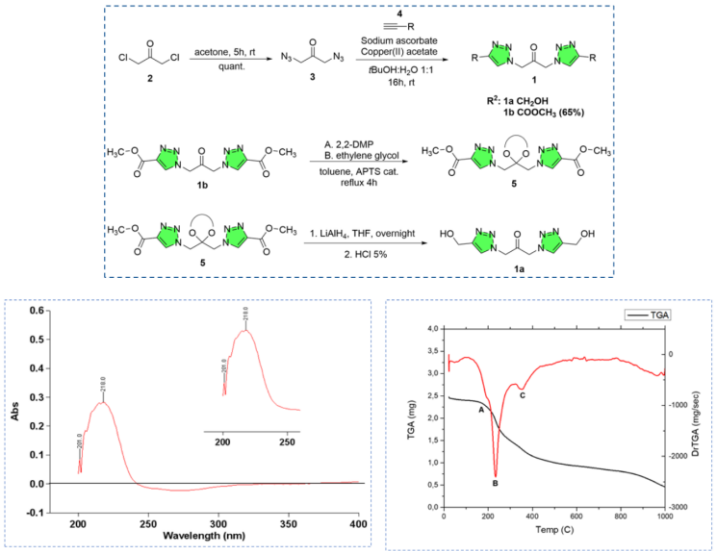
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Bistriazoles synthesis scheme; UV-Vis spectrum and TGA/DTG results.

Agradecimentos/Acknowledgments

UFBA, CAPES, GPSQ, LABCAT.

Synthesis of BORANIL-Thiadiazole Fluorophores

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Palavras Chave:*BORANIL,1,3,4-Thiadiazole,DSSC*

Highlights

Molecular hybrids containing the BORANIL and 1,3,4-Thiadiazole nuclei were synthesized in three steps with good yields.

Resumo/Abstract

Organic fluorescent dyes represent a class of materials with considerable potential owing to their broad applicability in diverse technological domains, including organic light-emitting diodes (OLEDs), dye-sensitized solar cells (DSSCs), chemosensors, bioimaging, lasers, and medical as well as pharmaceutical applications. In recent investigations, our research group has obtained promising results employing BORANIL derivatives in DSSCs.[1] Building upon these findings, we sought to conjugate the 1,3,4-thiadiazole group with the BORANIL nucleus in order to further enhance the optoelectronic properties of the resulting fluorophores. Thiadiazole-based structures have been extensively examined within the field of organic solar cells, as π-spacers in organic dyes, where they function as conjugated bridging units that extend absorption profiles and facilitate energy-level alignment with the TiO_2 surface, and as stabilizing elements that contribute to improved optoelectronic robustness of the sensitizer. In general, aryl aldehydes (1a-i) were reacted with thiosemicarbazide to give thiosemicarbazones (2a-i) which, by cyclization with ferric chloride, produced 2-amino-1,3,4-thiadiazole (3a-i). BORANIL-Thiadiazole derivatives (4a-i) were subsequently prepared by amidation of 2-amino-1,3,4-thiadiazole (3a-i) with benzoyl chloride (5), followed by complexation using $BF_3{\cdot}OEt_2$.[2] After purification by column chromatography, the products were obtained in yields ranging from 41% to 74%. In this study, the synthesis of nine molecular hybrids containing the new BORANIL-Thiadiazole (4a-i) were carried out in three steps with good yields.

[1] Leite, A. M. B.; et al.*Colorants*,**2024**,*3*, 311.
[2]Zhang, K.; et.al*Tetrahedron*,**2018**, 74, 4161.

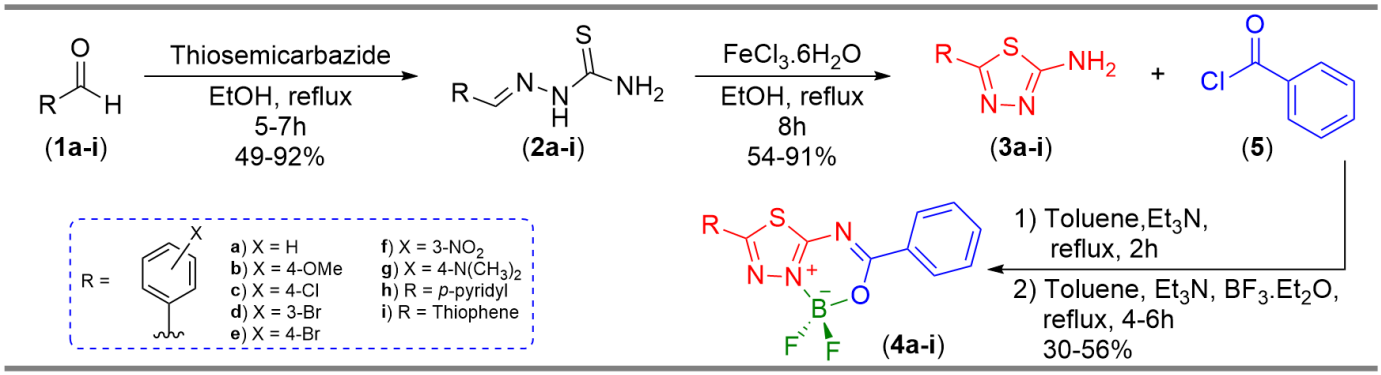


Figure 1. Synthesis of BORANIL-Thiadiazole fluorophores (4a-i).

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPERJ, UFF.

Synthesis of C6 Biaryl Derivatives of Chrysin

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[1]*Universidade Federal da Bahia*

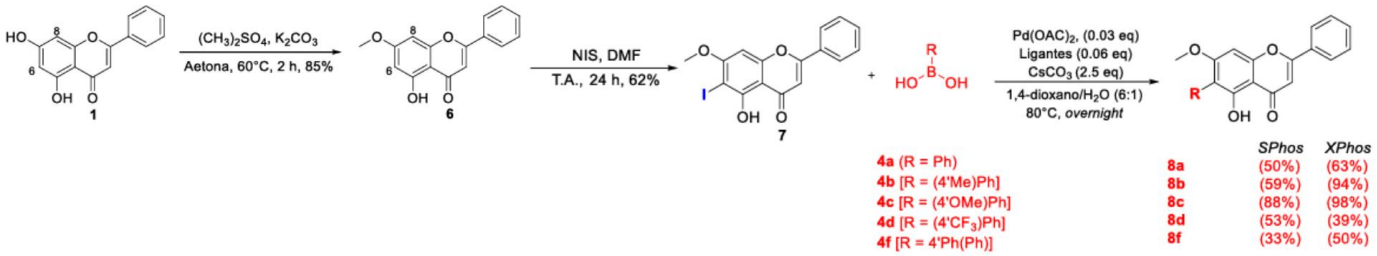
Palavras Chave:*Chrysin,Derivatives,Halogenation,Suzuki-Miyaura Cross-coupling*

Highlights

The focus of this research was to synthesize C_6 biaryl chrysin derivatives through Suzuki-Miyaura cross-couplings with commercial boronic acids.

Resumo/Abstract

Chrysin, belonging to the flavone class and an important group of flavonoids, underwent regioselective protection at the phenolic hydroxyl group at position C_7 using dimethyl sulfate, potassium carbonate in acetone at 60°C for 2 hours, with an 85% yield. Following this, the resulting compound was subjected to regioselective iodination at position C_6 using N-Iodosuccinimide (NIS) in N,N-Dimethylformamide (DMF) at room temperature (Souza, V. C.;*et al*,**2023**), with an estimated time between 24 and 48 hours, achieving a 62% yield after isolation on a chloroform chromatographic column. The classic Suzuki-Miyaura cross-coupling methodology, which consists of using palladium acetate ($Pd(OAC)_2$) (0.03 eq), ligands (0.06 eq), $CsCO_3$ (2.5 eq) in 1,4-dioxane/H2O (6:1) at 80°C overnight, was also successfully applied to the functionalization of chrysin at the C_6 position with commercial boronic acids, enabling the synthesis of five biaryl derivatives with yields ranging from 33 to 98%. Reactions carried out in the presence of the XPhos ligand showed superior results when compared to those conducted with SPhos for some of the products generated (Scheme 1). These products are being subjected to biological assays to evaluate the cell viability of Leishmania amazonensis promastigotes, as well as to investigate their interaction with alpha and beta estrogen receptors, aiming to expand their potential applications in the protection of the central nervous system. All molecules in this series are novel.



Scheme 1 - Synthesis of C6 of Chrysin

Agradecimentos/Acknowledgments

Fapesb, UFBA, Cienam, GPSQ, INCT, Capes, CNPq, PIBIC.

Synthesis of hybrids in triheterocyclic ring systems 4H-pyrimido[2,1-b]benzimidazole via MCR

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Palavras Chave:*heterocycles, green chemistry, and multicomponent reaction.*

Highlights

A derivative of 4*H*-pyrimido[2,1-*b*]benzimidazole, with potential to biological activities, was obtained through a multicomponent reaction and with an ionic liquid as catalyst.

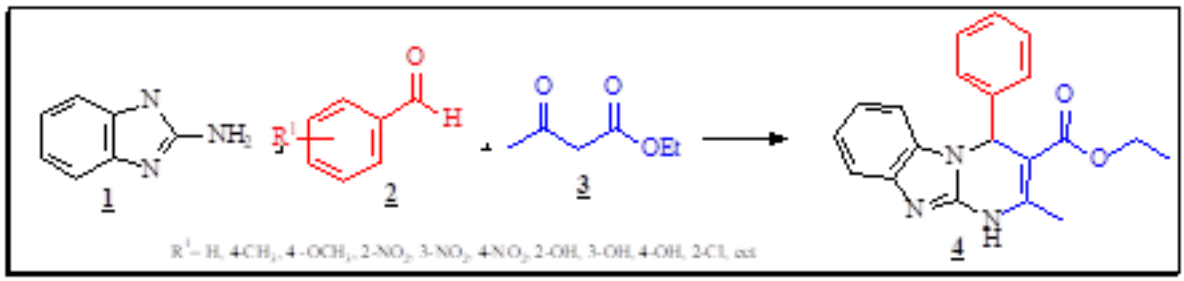
Resumo/Abstract

Benzimidazole and its derivatives are aromatic heterocyclic compounds that exhibit a broad spectrum of therapeutic activities, including antimicrobial, anticancer, antifungal, antileishmanial, and antituberculosis actions. Among the structurally modified subclasses, the substituted 2-aminobenzimidazoles stand out, which have been employed as novel inhibitors of acetylcholinesterase and butyrylcholinesterase enzymes, in addition to acting as potent glucagon receptor antagonists.[1] Due to this pharmacological and biological relevance, the present work aims at the synthesis of benzimidazole hybrids through multicomponent reactions (MCRs) in ionic liquids, aiming at the development of an efficient synthetic strategy that allows the obtaining of structurally complex molecules, with high atom economy, reduction in the number of reaction steps, minimal waste generation, and alignment with the principles of green chemistry.[2] In the synthesis of 4H-pyrimido[2,1-*b*]benzimidazole hybrids**4**(Scheme 1), a round-bottom flask adapted for reflux was used, where 1 mmol of 2-aminobenzimidazole**1**, 1 mmol of aldehyde**2**and 1 mmol of ethyl acetoacetate**3**were added under constant temperature and magnetic stirring. The synthesis of 4H-pyrimido[2,1-*b*]benzimidazole hybrids proved efficient with yields of 45-93%. It was possible to apply a synthesis with a catalyst and solvent with low toxicity that fits within the parameters of Green Chemistry, since the synthesis of this class of compounds has immense biological and pharmacological applicability.

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Scheme 1. Synthesis of a benzimidazole derivative.

Agradecimentos/Acknowledgments

We are frateful to CAPES, CNPq, FINEP, FAPEG and UEG

Synthesis of key precursors for the preparation of new molecular hybrids

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Palavras Chave:*4-Aminoquinazolines,Bioactive molecules,4-chlorocoumarins,Molecular hybrids*

Highlights

Quinazolines and coumarins are privileged compounds in medicinal chemistry.

We have studied the synthesis of 4-aminoquinazolines and 4-chlorocoumarins, which are precursors of new molecular hybrids.

Resumo/Abstract

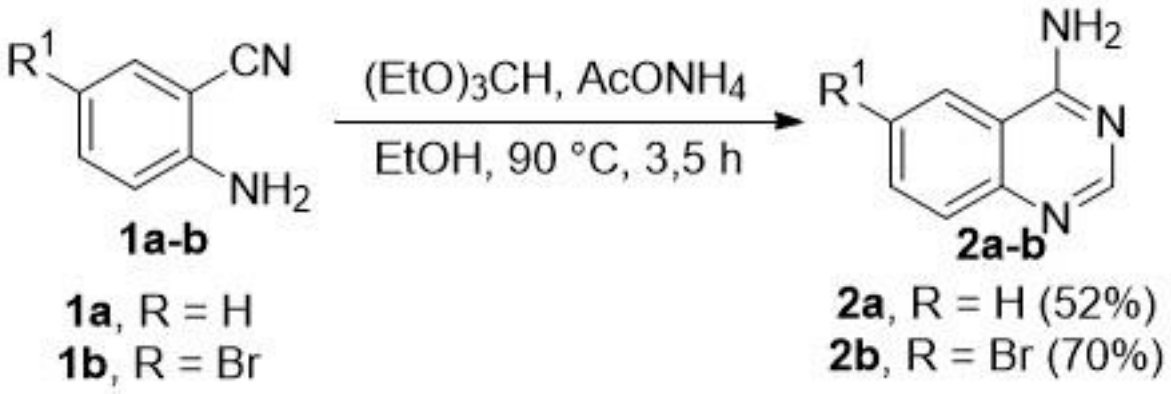
4-Aminoquinolinazolines and coumarins are privileged scaffolds in medicinal chemistry, since their structure may be found in compounds with several biological activities.[1,2] Thus, in this work, we have investigated the synthesis of 4-aminoquinazolines and 4-chlorocoumarins, which are key intermediates for the preparation of new molecular hybrids with potential biological activities. Initially, we performed the bromination of 2-aminobenzonitrile (**1a**) using*N*-bromosuccinimide in CH_3CN at 25 °C for 30 min, which allowed us to obtain 5-bromo-2-aminobenzotrile (**1b**) in 83% yield.[3] Subsequently, 4-aminoquinazolines (**2a-b**) were synthesized by the cyclocondesantion reaction between 2-aminobenzonitriles (**1a**or**1b**) and triethyl orthoformate in a basic medium, leading to the respective products in 52 and 70% (Scheme 1).[4] Currently, we are investigating the preparation of 4-chlorocoumarin from 4-hydroxycoumarin. In preliminary tests, we evaluated a methodology that promotes chlorination using a mixture of PPh_3/Cl_3CCN, but in all tests we afforded a mixture of the desired product with a dichlorinated byproduct.[3] In summary, we were able to prepare two 4-aminoquinazolines (**2a-b**) in good yields, which were characterized by NMR analysis. Furthermore, to achieve our objectives, further studies aimed at developing the best methodology for preparing 4-chlorocoumarins are currently being investigated in our research group.

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Scheme 1

Agradecimentos/Acknowledgments

CNPq, FACEPE and iCEIS.

Synthesis of N-ethyl 4-quinolone-3-carboxamides and evaluation of their antiproliferative activity against cervical cancer cells

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Palavras Chave:*4-Quinolone-3-carboxamides; N-alkylation; Antiproliferative activity; HeLa cells; ADMETox.,4-Quinolone-3-carboxamides; N-alkylation; Antiproliferative activity; HeLa cells; ADMETox.*

Highlights

Twelve 4-quinolone-3-carboxamides**1a-j**were synthesized, with a yield of 58-86%. The derivatives were evaluated for their antiproliferative activity against HeLa cells and favorable*in silico*ADMETox.

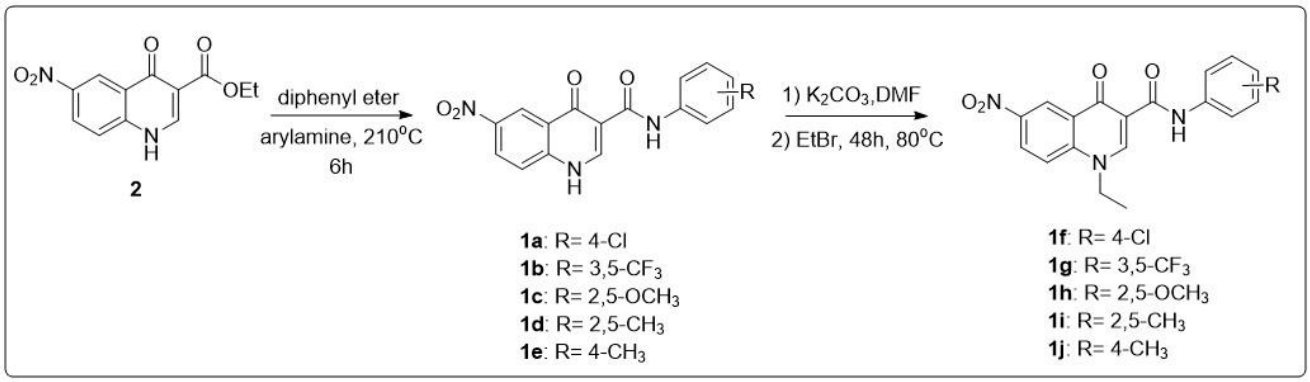
Resumo/Abstract

Cervical cancer remains a major global health challenge, ranking among the leading causes of cancer-related mortality in women, while therapeutic resistance and dose-limiting side effects continue to compromise current treatments. In this context, 4-quinolone-3-carboxamides have emerged as a privileged scaffold in medicinal chemistry due to their broad spectrum of biological activities. Herein, we report the synthesis, structural characterization, and antiproliferative evaluation of twelve novel 4-quinolone-3-carboxamide derivatives (**1a–j**). The synthetic strategy is based on a nucleophilic substitution at the C-3 carbonyl group of 6-nitro-4-oxoquinoline**2**using structurally diverse anilines, enabling efficient access to the target amides in overall yields ranging from 58 to 86%. Selected derivatives were further subjected to*N*-ethylation under mild conditions, affording*N*-ethyl-4-quinolone-3-carboxamides after purification by hot ethanol washing. All compounds were fully characterized by standard spectroscopic techniques.

The antiproliferative activity of the synthesized compounds was assessed against HeLa cervical cancer cells using the MTT assay. Cell cycle distribution and apoptosis induction at IC_{50} concentrations were investigated by flow cytometry, providing mechanistic insights into their biological effects. In parallel,*in silico*ADMETox simulations were performed to estimate pharmacokinetic behavior and toxicity risks. Among the evaluated compounds, derivatives**1b**(IC_{50} = 11.35 µM) and**1i**(IC_{50} = 21.68 µM) displayed the most pronounced antiproliferative effects, with LT12 exhibiting a high selectivity index (SI > 9). These results highlight the synthetic versatility of the proposed approach and identify*N*-ethyl 4-quinolone-3-carboxamides as promising leads for further optimization toward novel agents for cervical cancer therapy.

1-*World Health Organization. Cancer in 2025. WHO; 2026.*

2-*Forezi LSM, et al.Eur J Med Chem. 2020;194:112255.*



Scheme 1. Synthetic methodology for the preparation of N-ethyl-4-quinolone-3-carboxamides 1a–j.

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES (Código de Financiamento 001)

Synthesis of new 1,2,3-triazolyl-4-quinolone derivatives as potential antiviral agents

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Palavras Chave:*quinolones,triazoles,antiviral,synthesis*

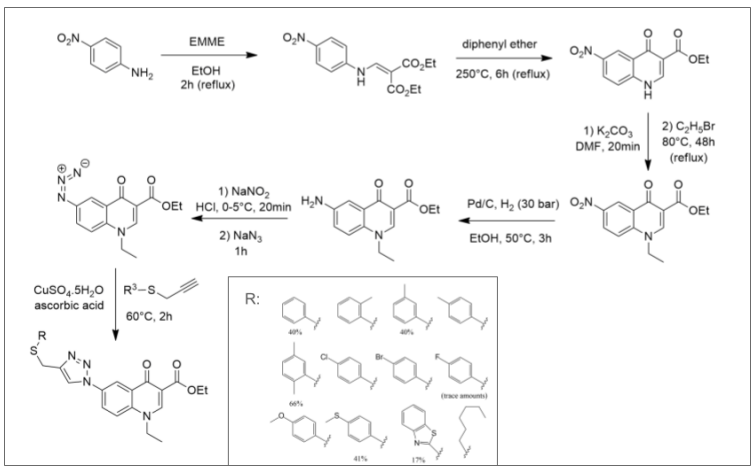
Highlights

The increasing resistance of viral strains poses a major public health threat
Hybrid quinolone–triazole derivatives emerge as potential antiviral agents
New compounds were synthesized and characterized

Resumo/Abstract

The increasing resistance of viral strains has become a major challenge for public health worldwide, driving a continuous search for new compounds with antiviral activity. The emergence of multidrug-resistant variants compromises the effectiveness of the currently available treatments, emphasizing the urgent need for innovative strategies to effectively control viral infections. In this context, hybrid derivatives of 4-quinolones and triazoles stand out as promising candidates for the development of new agents with potential antiviral activity, due to their structural versatility and capacity for effective interaction with biological targets.

Therefore, the present study focuses on the synthesis and characterization of a series of new hybrid 4-quinolone-triazole derivatives with the purpose of investigating their antiviral potential. The proposed strategy is based on the synthesis of compounds bearing a 4-quinolone core strategically functionalized at positions 1, 3 and 6: an ethyl group at position 1, an ethyl ester group at position 3 and a triazole ring at position 6, with different sulfur-containing substituents attached.
At the present stage of this study, six final products have been successfully obtained and characterized by spectroscopic techniques, as well as all the intermediates of the synthetic route. The yields of the intermediates ranged from 61% to 78%, whereas the yields of the final products ranged from trace amounts to 66%. The next steps involve completing the synthetic route in order to obtain the remaining derivatives, followed by the characterization of the synthesized compounds and the evaluation of their biological activity.



Proposed synthetic route for the synthesis of 4-quinolone derivatives starting from 4-nitroaniline.

Agradecimentos/Acknowledgments

Support from SiMIB, PPGQ and FAPERJ is gratefully acknowledged.

Synthesis of new 4-Quinolone-3-Hydroxamic Acid Derivatives and Evaluation of Their Anti-HSV-1 Activity

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Palavras Chave:*4-Quinolones,Hydroxamic acids,N-alkylation,Antiviral activity,HSV-1*

Highlights

New 4-quinolone-3-hydroxamic acid derivatives were synthesized and characterized, showing anti-HSV-1 activity with low cytotoxicity and supporting C-3 functionalization as a viable antiviral strategy.

Resumo/Abstract

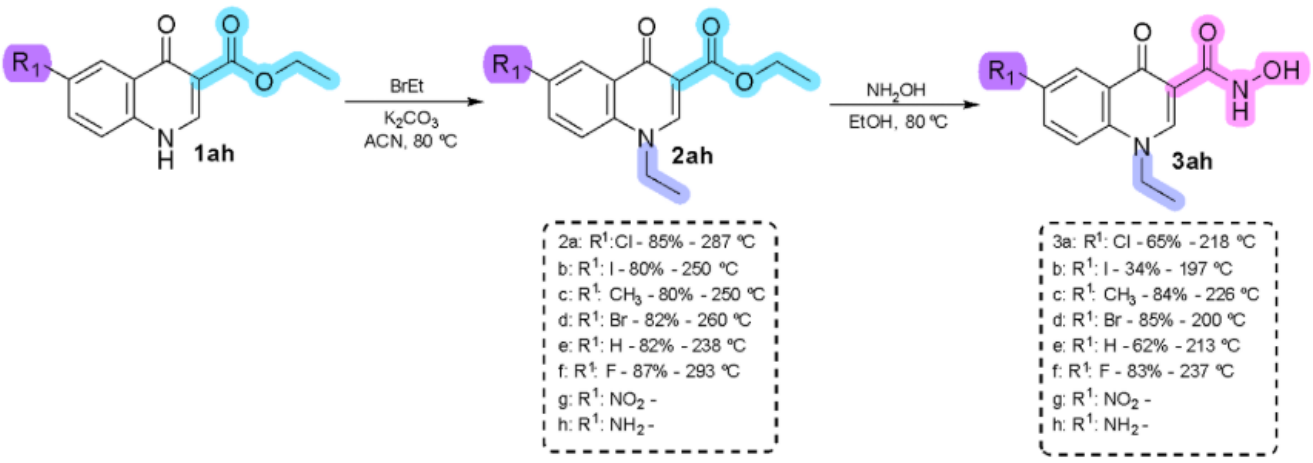
Herpes simplex virus type 1 (HSV-1) infections remain a relevant public health concern, particularly due to the emergence of viral strains resistant to standard antiviral therapy such as acyclovir. In this context, the 4-quinolone scaffold has been recognized as an important molecular structure in medicinal chemistry, while hydroxamic acids are well-known for their ability to chelate metal ions involved in essential viral enzymatic processes. In the present study, a series of new 4-quinolone-3-hydroxamic acid derivatives was designed and synthesized to explore the combined contribution of the quinolone core and the hydroxamic acid functionality to antiviral activity. The synthetic route involved thermal cyclization to construct the 4-quinolone nucleus, followed by N-alkylation and subsequent nucleophilic substitution at the C-3 carbonyl group using hydroxylamine generated in situ from $NH_2OH{\cdot}HCl$ and KOH. This strategy enabled efficient access to seven unprecedented hydroxamic acid derivatives in isolated yields ranging from 34 to 83%. All compounds were fully characterized by IR, ^1H and ^{13}C NMR spectroscopy, high-resolution mass spectrometry, and melting point analysis. The antiviral activity of the synthesized compounds was evaluated against HSV-1, and cytotoxicity was assessed in parallel. The derivatives displayed inhibition of viral replication ranging from 3.25% to 42.27%, while maintaining low cytotoxicity profiles (CC_{50} > 300 µM). Although moderate, these results indicate that functionalization of the 4-quinolone core with a hydroxamic acid moiety at the C-3 position is a viable synthetic strategy and provides a promising framework for further structural optimization toward more potent anti-HSV-1 agents.

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2) Richter, S., et al. Infectious disorders, 2004.

3) LV, W., et al. Frontiers in Pharmacology, 2025.



Synthetic methodology for obtaining 4-Quinolone-3-Hydroxamic Acid Derivatives 3ah

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES (Finance Code 001)

Synthesis of new triazolyl-chromone derivatives with anti-protozoal profile

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Palavras Chave:*Chromone,Triazole,anti-protozoal,Heterocycles,Anti-protozoal*

Highlights

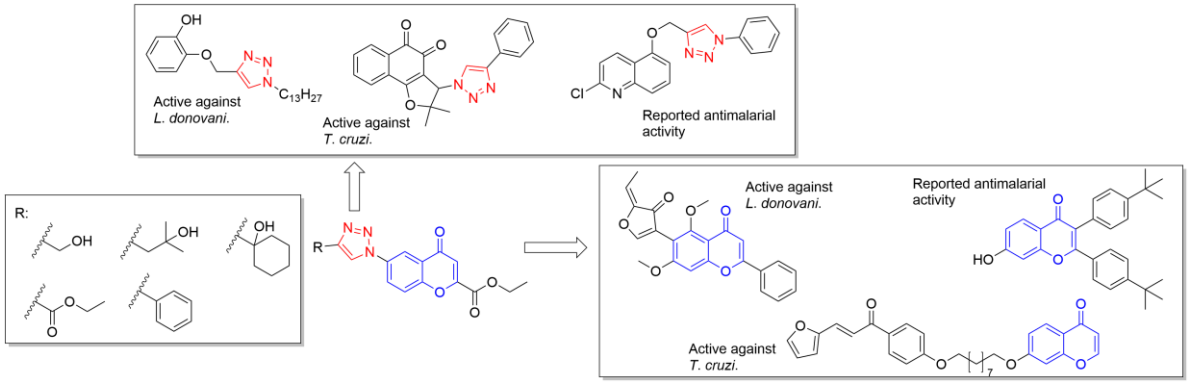
Development of a new class of triazole/chromone chromone hybrids for anti-protozoal activity. Synthesis of 6-(triazolyl)chromone derivatives as new potential agents with anti-protozoal profile.

Resumo/Abstract

Protozoan infections are diseases caused by organisms that can act as parasites in mammals and humans, affecting various systems, especially the gastrointestinal system. Notable infections include Malaria, Leishmaniasis, Chagas disease and Human African Trypanosomiasis, affecting hundreds of millions worldwide and causing from gastrointestinal disturbances, skin lesions to death in severe cases. These diseases are mostly prevalent in tropical developing countries such as Brazil, which had close to fifteen thousand deaths caused by Malaria, Leishmaniasis and Chagas in 2024. Current treatments for these diseases are associated with high toxicity and severe side effects, highlighting the urgent need for development of new drugs targeting these infections. Chromones are a class of heterocyclic compounds characterized by a benzene fused with a 4*H*-pyranone ring and is present in a variety of natural products. Chromones present several biological applications, including anti-protozoal as reported by different research groups. The 1,2,3-triazole nucleus consists of a five-membered heterocycle with three adjacent nitrogens, being an electron-rich aromatic system and can form complexes with an array of enzymes and biological receptors through intermolecular interactions, including in several protozoan species.

So far 4 synthetic intermediates have been synthesized and characterized, 2 of the final triazolyl chromone derivatives have been synthesized and have yet to be purified and characterized. As a prospect, the remaining substances will be synthetized and once obtained, their structures will also be elucidated using spectroscopic methods and, subsequently, they will be subjected to anti-protozoal biological activity assays, in collaboration with the research groups of Prof. Dr. Marcela Cristina de Moraes (GQO-UFF) and Dr. Luzineide Wanderley Tinoco (IPPN-UFRJ).

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Structure of final products and reported compounds with anti-protozoal activity

Agradecimentos/Acknowledgments

CNPq, FAPERJ, PPGQ-UFF, PROAP-UFF, CNPq-PIBIC, CAPES (Finance Code 001).

Synthesis of novel 9-amino-α-xyloidones with potential antineoplastic properties

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Palavras Chave:*dehydro-α-lapachones,cancer,α-caryopterone,regioselective synthesis,bioisosterism*

Highlights

Naphthoquinones bearing an amino group on the aromatic ring have been scarcely explored. In this work, we report the synthesis of structurally novel 9-amino-α-xyloidones with antineoplastic potential.

Resumo/Abstract

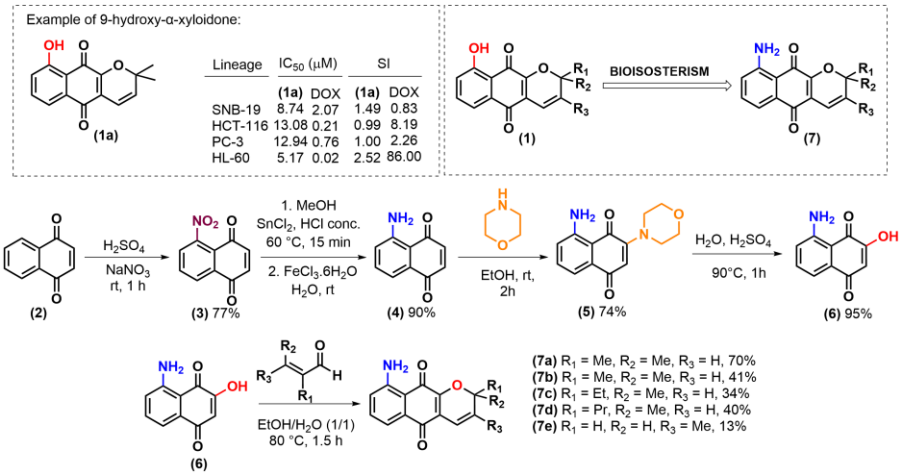
Naphthoquinones are a class of compounds extensively studied due to their wide range of biological activities, although relatively few investigations have focused on modifications of their aromatic ring.[1] Pyranonaphthoquinones hydroxylated on the aromatic ring**(1)**have been reported as promising antineoplastic agents.[2] Naphthoquinones bearing aromatic amino groups constitute a class of molecules with considerable biological potential that remains poorly explored in the literature. In this context, the present study aims to generate bioisosteres of hydroxy-α-xyloidones by replacing the hydroxyl group with an amino group, in order to evaluate the impact of this modification on their biological activity. The synthetic route employed (Scheme 1) began with the nitration of 1,4-naphthoquinone**(2)**, affording the nitrated intermediate**3**, which was subsequently reduced to yield compound**4**.[3] The resulting aminated intermediate underwent an aza-Michael addition with morpholine, producing compound**5**regioselectively. Subsequent hydrolysis afforded 8-aminolausone**(6)**.[4] Finally, a Knoevenagel condensation followed by electrocyclization with α,β-unsaturated aldehydes yielded five novel 9-amino-α-xyloidones**(7)**.[2] The antitumor activity of these compounds is currently under investigation.

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Scheme 1. Planning and synthetic route for the production of naphthoquinones 7. DOX, doxorubicin

Agradecimentos/Acknowledgments

PPGQ-UFF, FAPERJ, CAPES, and CNPQ

Synthesis of Novel Schiff Base Phosphoramidates. A reaction via Schif amino-base intermediates.

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Palavras Chave:*Phosphoramidate,Schiff bases,biological activity,metal complexing agent.*

Highlights

This work proposed the synthesis of a series of novel phosphoramidates derived from Schiff bases and evaluated their biological capabilities against strains of pathogenic microorganisms.

Resumo/Abstract

In 1864, Hugo Schiff was the first to synthe Schiff bases, using aldehyde or ketone and a primary amine. These Schiff bases can be considered a subclass of imines with a general structure R1R2C=NCR3. Schiff bases have a wide range of biological properties, notably, as antimicrobial, anticancer, antiviral, antimalarial, antioxidant, anti-inflammatory, antifungal agents, possess antiproliferative, analgesic, and antipyretic properties.In turn, organophosphorus compounds are key substrates in the design of drugs and prodrugs. Predominantly, phosphoramidates (P-N) belong to a class of organophosphorus compounds, known for the presence of a single covalent bond between the tetracoordinated P(V) atom and the N(III) atom. Thus, the phosphoramidate skeleton, which plays a strategic biological role and is therefore an interesting model for combinatorial and medicinal chemistry, and be able to coupled with other portions of recognized medicinal activity. In this way,can be it becomes a new therapeutic concept available to society.This work aimed to synthe new Schiff base phosphoramidates (5) using two synthesis routes. The first route (A) involves obtaining the reaction intermediate 3, called Schiff amino-base. This stage of the work (route A) is practically complete (Figure-1) and describes the strategic mono-condensation reaction of aromatic diamines with substituted aldehydes and benzaldehyde.Thus, to obtain 3, the conditions of Ajima et al (Figure-1) were applied. so far, we have been able to synthe the Schiff 3a-e amino-base intermediates. The derivatives showed different reaction times, due to the structural relationships between the reagents (Table-1). Preliminary reactions of phosphorylation of the free amino group of 3 are in implementations (route B), (Figure-1) and are initially planned via the methodology of Zhao et al, using dibutyl phosphite (4) in biphasic medium. All synthed derivatives (3) were confirmed by IR, 1H and 13C NMR spectroscopic techniques.

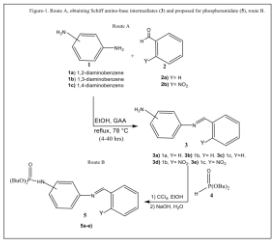


Table 1. Reaction time and physical properties of 3

Compound	Reaction Time	Melting point	Yield	Coloring
3a	40 hrs	139 °C	52%	yellow
3b	8hrs	187 °C	72%	light yellow
3c	8hrs	139 °C	78%	light beige
3d	4hrs	91 °C	69%	reddish yellow
3e	4hrs	234 °C	70%	red

Route for obtaining Schiff amino-base derivatives (3a-e) and methodological proposal for the 5.

Agradecimentos/Acknowledgments

To the Analytical, Innovation and Technology Center of UEG (CAITEC). To Prof. Dr. Luciano Morais Lião-UFG for the analyses (Nuclear Magnetic Resonance Laboratory) To the State University of Goiás for the structure of our Research Group, GPO-UEG.

Synthesis of porphyrins linked to 1,2,3-triazole derivatives for the study of their biological activity and applications.

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[1]Universidade Federal da Bahia

Palavras Chave:*Porphyrins,CuAAC reaction,triazole derivatives*

Highlights

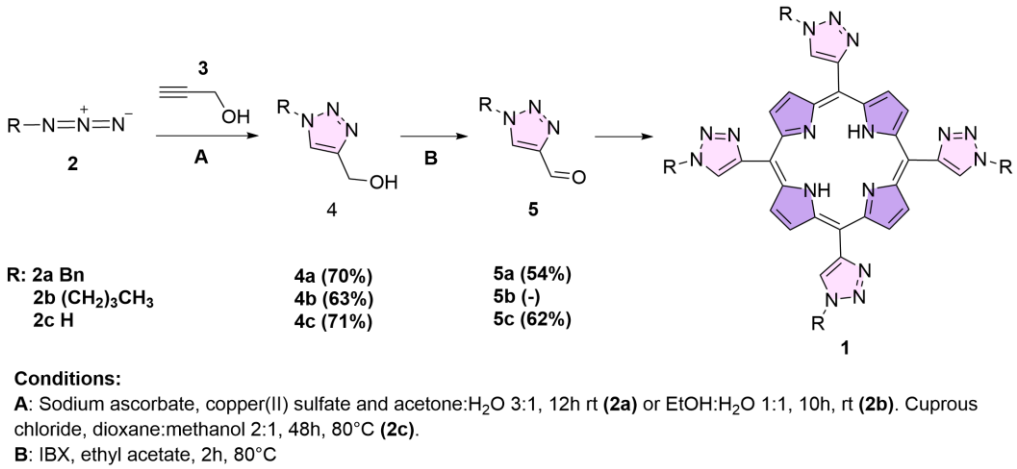
Synthesis of triazole-linked porphyrins. Synthesis of 1,2,3-triazole derivatives via CuAAC reaction. Study of the biological activity of triazole-linked porphyrins.

Resumo/Abstract

In recent decades, triazoles have been studied for their potential applications in medicinal chemistry due to their biological activities as neuroprotective agents, leishmanicidal agents, antivirals, and in other diseases. Research has examined the effects and use of these compounds in various areas when linked to porphyrins, which are heterocyclic organic substances essential for oxygen transport and storage in hemoglobin and muscles, and have been studied for cancer treatments and other uses in medicine. In this context, this work aims to synthesize three derivatives of 1,2,3-triazoles via CuCAAC reaction, couple them to porphyrins, and study their biological activities. Initially, the triazoles were synthesized in their alcohol forms (3), and then oxidized to their corresponding aldehydes (4). To obtain the aldehyde of triazole 3a, oxidation methods using manganese dioxide (MnO2), pyridinium chlorochromate (PCC), and 2-iodobenzoic acid (IBX) were tested; however, only the IBX method was effective and applied to the other two triazoles. Although aldehydes 4a and 4c were successfully isolated and characterized by infrared spectrometry, the aldehyde 4b proved unstable, being very sensitive to temperature during purification, and it has not yet been possible to obtain it in isolated form. We're looking forward to completing the synthesis of all three aldehyde triazoles and linking them to the porphyrins.

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V. S. Pore, S. G. Agalave, S. R. Maujan.*Chem. - An Asian J.***2011,**6, 10, 2696-2718



Scheme 1. Obtaining of porphyrins 1

Agradecimentos/Acknowledgments

UFBA, GPSQ

Synthesis of Quinolone-Based Acyclonucleoside Isobutyrate Prodrugs with Antiviral Activity against SARS-CoV-2

Thiago Mota do Vale (PG)[1], Maria Fernanda Rosa Nunes (IC)*[1], Letícia Villafranca Faro (PQ)[1], Pedro Netto Batalha (PQ)[1], Mayara Mattos da Conceição (PQ)[2], Lina Marcela Silva Trujillo (PQ)[2], Caroline Souza de Freitas (PQ)[2], Natalia Fintelman-Rodrigues (PQ)[2], Maria Cecilia Bastos V. de Souza (PQ)[1], Thiago Moreno Souza (PQ)[2], Fernanda da Costa Santos Boechat (PQ)[1].

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Palavras Chave:*Acyclonucleosides; 4-Quinolones; Prodrugs; Isobutyrate esters; SARS-CoV-2*

Highlights

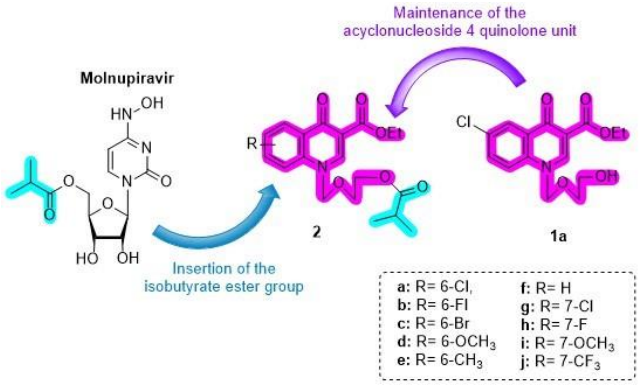
New quinolone-based acyclonucleoside prodrugs were synthesized by a one-pot strategy, with higher antiviral potency after isobutyrate esterification and high SARS-CoV-2 inhibition in two cell models.

Resumo/Abstract

Despite the official declaration of the end of the COVID-19 pandemic, the continuous emergence of new SARS-CoV-2 variants sustains the need for the development of novel antiviral agents. In this context, quinolone-based acyclonucleosides represent a promising class of compounds, combining a privileged heterocyclic scaffold with structural features associated with antiviral activity. In the present study, a known quinolone acyclonucleoside derivative previously reported as active against HSV was selected as a lead structure for the design of a new and unprecedented series of quinolone-based acyclonucleoside isobutyrate prodrugs (**2a–j**).

The synthetic route involved the preparation of the parent acyclonucleosides (**1a–j**) from appropriately substituted 4-quinolones via a one-pot procedure comprising an initial silylation step followed by the addition of 1,3-dioxolane. Subsequent introduction of the isobutyrate moiety was achieved by reaction with isobutyric anhydride, affording the target prodrugs in satisfactory yields. All compounds were fully characterized by standard spectroscopic methods. The antiviral activity of both series (**1a–j**and**2a–j**) was evaluated against SARS-CoV-2 in HuH-7 and Calu-3 cell lines. Several derivatives displayed pronounced inhibition of viral replication, with compounds**1c**,**2e**,**2h**and**2j**showing ≥ 80% inhibition in HuH-7 cells, while compounds**2a**,**2b**,**2c**,**2d**,**2g**,**2h**and**2j**reached similar inhibition levels in Calu-3 cells. Overall, the incorporation of the isobutyrate ester proved to be a relevant structural modification, consistently enhancing antiviral potency across both cellular models and supporting the prodrug strategy as an effective approach for the optimization of quinolone-based acyclonucleosides against SARS-CoV-2.

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3-**Lucero BD et al.**Quinolonic acyclovir analogues.*Bioorg Med Chem Lett.*, 2006



Scheme 1. Synthetic design for the preparation of quinolone-based acyclonucleoside isobutyrates 2.

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES (Código de Financiamento 001)

Synthesis of Quinolone Carboxamide-Based Acyclonucleosides as Potential Anti-HSV-1 and HSV-2 Agents

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Palavras Chave:*HSV,Antiviral,4-Quinolona,Carboxamida,Aciclonucleosídeos*

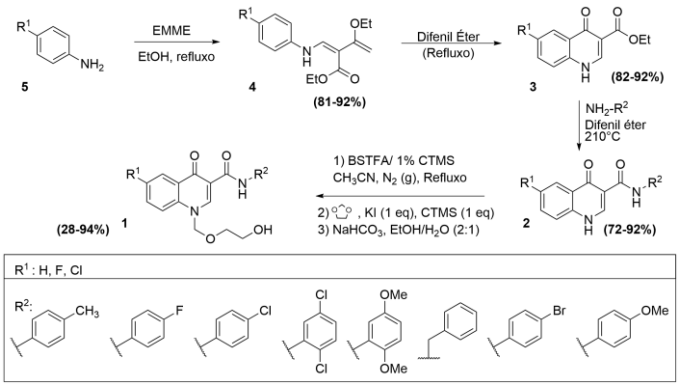
Highlights

Quinolone-3-carboxamide-based acyclonucleosides were synthesized via an adapted Vorbrüggen strategy, affording a broad yield range and targeting antiviral activity against HSV-1 and 2.

Resumo/Abstract

Herpes simplex viruses type 1 and type 2 (HSV-1 and HSV-2) are widespread human pathogens and remain a significant public health concern due to their high transmissibility, lifelong persistence, and potential development of resistance to currently available antiviral therapies. Although nucleoside analogues such as acyclovir are effective in reducing the severity and duration of clinical episodes, the absence of curative treatments highlights the need for new antiviral agents with improved profiles. In this context, nucleoside-inspired structures have emerged as valuable scaffolds due to their ability to interfere with key enzymatic steps in viral replication. In the present work, we describe the synthesis of a new series of acyclonucleoside derivatives incorporating a quinolone-3-carboxamide core, designed to combine the pharmacological relevance of the quinolone scaffold with structural features characteristic of antiviral nucleosides. The target acyclonucleosides (1) were synthesized from their corresponding 4-quinolone-3-carboxamide precursors (2) using an adapted Vorbrüggen methodology, as outlined in Scheme 1. This synthetic strategy enabled the efficient construction of the acyclic nucleoside framework, affording the desired compounds in isolated yields ranging from 28 to 94%. All derivatives were obtained through reproducible procedures and are currently undergoing full structural characterization by standard spectroscopic techniques. Following synthesis and characterization, the compounds will be evaluated for their antiviral activity against HSV-1. The results of this study are expected to contribute to the development of quinolone-based acyclonucleosides as promising candidates for further optimization in the search for new anti-HSV agents.

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[2] Amorim, L. S. C.; STEPHENS; P. R. S.; et al, Braz. J. Pharm. Sci, 2026.
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Scheme 1. Synthetic route for the preparation of quinolone carboxamide-based acyclonucleosides.

Agradecimentos/Acknowledgments

CNPq, FAPERJ, CAPES (Finance Code 0001)

Synthesis of retusine analogs via the Suzuki-Miyaura reaction, with potential anti-Chikv activity.

Andréia de S. Maller Sanchez (PG)*[1], Nathália Santos de Oliveira (PG)[1], Edgar Schaeffer (PQ)[1], Luana G. de Souza (PQ)[2], Louise de A. Carvalho (IC)[1], Alcides J. M. da Silva (PQ)[1].

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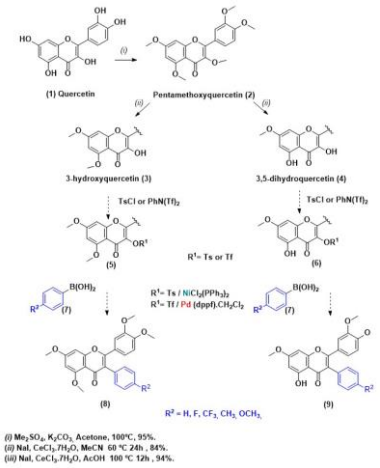
Palavras Chave:*SYNTHESIS,CATALYSIS,FLAVONOIDS,RETUSINE*

Highlights

• A synthetic strategy starting from quercetin was developed to access novel C-3 arylated flavonoids.
• The designed flavonoid derivatives are proposed as potential antiviral agents against CHIKV.

Resumo/Abstract

The chikungunya virus (CHIKV) is an arbovirus from the Alphavirus genus transmitted mainly by the mosquitoes Aedes aegypti and Aedes albopictus. Its rapid and efficient replication cycle makes several stages attractive targets for antiviral drug development (WEAVER; FORRESTER, 2015). In this context, flavonoids have attracted increasing scientific interest due to their broad spectrum of biological activities. Among them, quercetin stands out as a flavonol widely distributed in nature with a well-established pharmacological profile. Phenolic derivatives of quercetin have been reported as potential inhibitors of viral replication, including CHIKV (LI et al., 2016; FERRAZ et al., 2023). Structural studies indicate that flavones bearing specific substitution patterns in the flavonoid core, particularly at C-3 and C-5, may display antiviral activity against arboviruses.
Within this framework, retusin emerges as a representative compound of this class. This methoxyflavonol occurs naturally in plant species, especially citrus fruits, and has been associated with relevant biological properties (MANTHEY; GUTHRIE, 2002). Preliminary studies from our group indicated that the derivative 3-OH-retusin showed evidence of viral replication inhibition, motivating the design of a new series of C-3 arylated flavonoids through Suzuki–Miyaura cross-coupling reactions.
As illustrated in Scheme 1, the synthetic route starts from quercetin (1), initially subjected to permethylation with Me_2SO_4, affording pentamethoxyquercetin (95%). Subsequent selective demethylation using NaI/$CeCl_3$•$7H_2O$ provided 3-hydroxyquercetin (3) in MeCN at 60 °C for 24 h (84%) and 3,5-dihydroxyquercetin (4) in AcOH under reflux for 12 h (92%). The hydroxyl group at C-3 will then be converted to triflate (OTf) or tosylate (OTs), generating pseudohalides suitable for Suzuki–Miyaura coupling with arylboronic acids (7) to afford novel 3-arylflavones and 3,5-arylflavones (8,9).



Scheme 1. Synthetic strategy for obtaining arylated flavonoids in C-3

Agradecimentos/Acknowledgments

CAPES, CNPQ, FAPERJ, IPPN, UFRJ

Synthesis, Structural Characterization, DFT Studies, and Phytotoxic Evaluation of Novel Tetronamides Derived from Mucobromic Acid

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Palavras Chave:*Tetronamide,mucobromic acid,menthol,herbicide,theoretical calculations*

Highlights

Tetronamides derived from mucobromic acid and menthol were synthesized.

Compounds were characterized by spectroscopic methods and DFT.

All compounds exhibited significant phytotoxic activity.

Resumo/Abstract

Tetronamides are β-amino-substituted butenolide heterocycles with a conjugated system and high reactivity. In the search for new herbicides, six tetronamides were synthesized from mucobromic acid and menthol. The acyclic form of mucobromic acid was activated by (1*S*)-(+)-10-camphorsulfonic acid (CSA), enabling the enantioselective synthesis of compound 1, which was used as a precursor in the aza-Michael addition/elimination reaction on the butenolide ring (Figure 1).The first step consisted of reacting mucobromic acid with (-)-menthol in toluene under reflux with a Dean–Stark apparatus for 24 h. After extraction and chromatography, the product was reacted with various anilines in DMSO at room temperature for 24 h. The resulting compounds were isolated by extraction and purified on silica gel, leading to the formation of the new tetronamides 2–7. The molecular structures were elucidated using spectroscopic techniques such as IR, NMR, and mass spectrometry, supported by theoretical calculations based on Density Functional Theory (DFT). The phytotoxic activity of these compounds was also investigated against species such as*Cucumis sativus*,*Solanum lycopersicum*,*Sorghum bicolor*,*Urochloa brizantha*, and*Bidens pilosa*. The assays indicated a significant reduction in root and shoot growth for most of the tested compounds, with root inhibition exceeding 60% at a concentration of 300 µM. The relative configuration of the chiral centers was determined as SRSR based on spectroscopic analyses, computational calculations, and probabilistic methods, including DP4, DP4+, Linear Regression (R^2), and Corrected Mean Absolute Error (CMAE).

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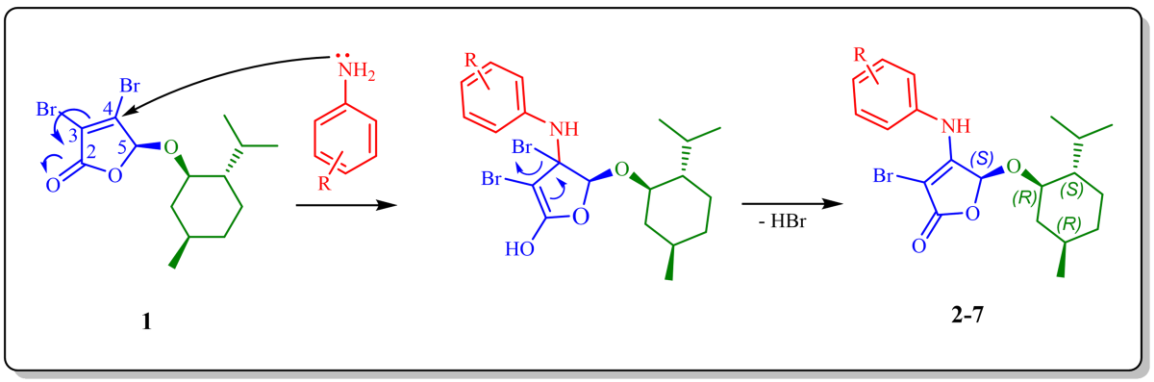


Figure 1. Mechanistic proposal for obtaining new tetronamides 2-7

Agradecimentos/Acknowledgments

FAPEMIG, CNPq, CAPES, UFV

Trichloroisocyanuric Acid (TCCA) from pool sanitation as a chlorination reagent for thymol

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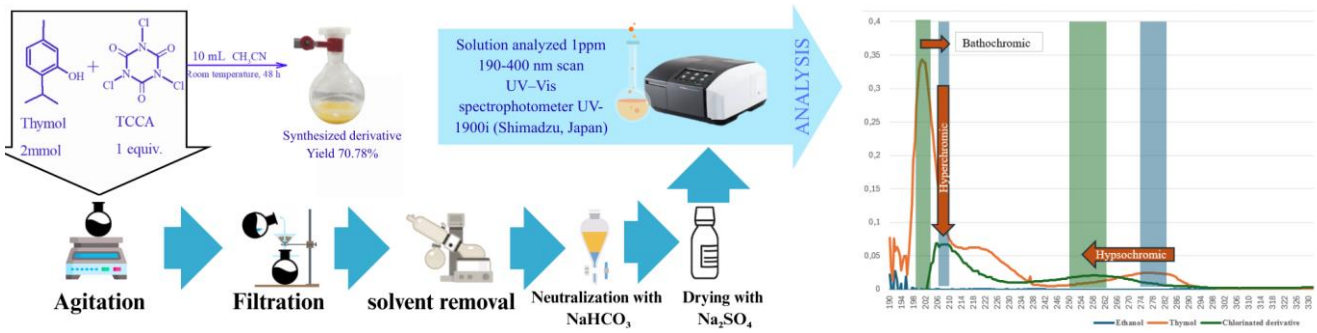
Palavras Chave:*Halogenation, Synthesis, Thymol, Trichloroisocyanuric Acid*

Highlights

TCCA used in pool sanitation was used as an alternative reagent to obtain a halogenated thymol derivative, focusing on applications of synthesis with alternative reagents.

Resumo/Abstract

Thymol is a natural phenolic monoterpene from essential oils such as*Thymus vulgaris*and*Origanum vulgare*, with anti-inflammatory, antibacterial, antioxidant, and antiseptic activities.[1,2] Functionalization of bioactive molecules is an efficient strategy in medicinal chemistry, and halogenated compounds are widely applied in pharmaceuticals and diagnostics.[3] Thus, this study aims to develop a synthetic route for chlorinated thymol derivatives using trichloroisocyanuric acid (TCCA), from pool sanitation. The methodology used and the results are presented in Figure. When the maximum absorptions were compared, the primary and secondary bands of the aromatic system in the derivative showed shifted values in relation to that of thymol. Aromatic rings such as that of thymol may exhibit three$\pi \rightarrow \pi^*$electronic transitions in the excited state, with primary bands at 180 and 202 nm and a secondary band at 255 nm. The introduction of substituents into the aromatic ring, regardless of electron-donating or electron-withdrawing character, shifts the primary band to higher wavelengths, from 202 nm in the reagent to 207 nm in the derivative, exhibits a bathochromic effect. Because this is a forbidden transition, the introduction of halogens (multiple chlorines) reduces the ring electron density, hindering the transition and decreasing peak intensity. In the secondary band, halogens disturb$\pi \rightarrow \pi^*$or$n \rightarrow \pi^*$conjugation, increasing transition energy and causing a hypsochromic shift from 279 nm to 258 nm in the derivative. Thus, UV-Vis analysis indicates that TCCA is a viable alternative for the synthesis of halogenated thymol results.
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Chlorination reaction and UV-Vis spectrum

Agradecimentos/Acknowledgments

I would like to thank the Essential Oils Laboratory (LOE) and the Organic Synthesis Laboratory (LABsínt) for their work, the UESB and CAPES for their financial support.

Understanding the Structure–Activity Relationship of Benzoxazole Derivatives as Anticancer Agents

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Palavras Chave:*cytotoxicity,heterocyclic,ketene dithioacetals,synthesis,vinylic substitution*

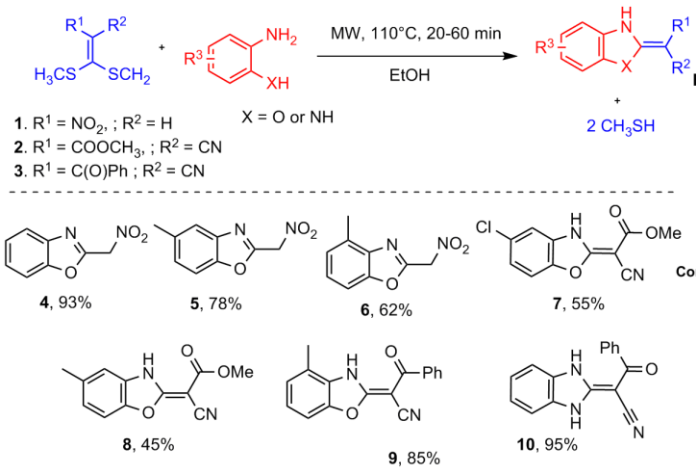
Highlights

Heterocyclic derivatives from ketene dithioacetals show selective cytotoxicity and apoptosis-related effects in human cancer cell lines, highlighting their potential as anticancer prototypes

Resumo/Abstract

Cancer comprises a broad group of diseases characterized by uncontrolled cellular proliferation and the ability to invade tissues and metastasize. Many drugs currently used in therapy exhibit low selectivity and significant toxicity toward healthy cells, reinforcing the need for the development of new antitumor prototypes.*N*-heterocyclic compounds are widely employed in the construction of molecular libraries for screening campaigns aimed at discovering new drugs. In a previous study, we synthesized a library of 19 nitrogen-containing heterocycles derived from ketene dithioacetals via double vinylic substitution, through which two benzoxazoles with noteworthy in vitro anticancer activity were identified, and in silico interaction with HDAC8. In the present work, we synthesized and evaluated the anticancer activity of additional benzoxazoles and benzimidazoles in order to investigate structure–activity relationships.The compounds were synthesized using substituted 2-aminophenols and o-phenylenediamine as nucleophiles in reactions with ketene dithioacetals. Seven heterocyclic compounds were synthesized and tested against seven cell lines, demonstrating that benzoxazole ylidenes substituted with cyano and benzoyl groups are active against THP1 cancer cells. In silico studies indicate that this activity is associated with interactions with the enzymes MMP9 and HDAC8. Benzoxazoles bearing different substitution patterns at the double bond, as well as the benzimidazole analogue with the same substituent, did not exhibit significant activity. Taken together, these findings support that heterocyclic ketene dithioacetal derivatives may display promising profiles of selectivity and target engagement, justifying further structural optimization and additional mechanistic and validation studies.1

1-. Synthesis and cytotoxic evaluation of heterocyclic compounds by vinylic substitution of ketene dithioacetals. Chemistry & Biodiversity, [s.l.], v. 21, e14581, 2024.



Binding energy values (kcal/mol)	HDAC8 (1W22)	MMP9 (1GKC)
4	-4.6	-7.3
5	-4.6	-7.8
6	-4.8	-7.5
7	-4.8	-8.3
8	-5.1	-8.4
9	-6.1	-9.5
10	-6.7	-9.3

Compound IC_{50} (μM)	MDA-MB-231	TOV-21G	A549	WI-26VA4	THP-1	K562	PBMC
4	>100	>100	>100	>100	>100	>100	>100
5	33.2	55.9	95.8	>100	>100	>100	>100
6	>100	>100	98.1	>100	>100	>100	>100
7	15.5	23.2	33.9	19.6	28.1	>100	>100
8	54.2	>100	48.7	>100	44.1	>100	>100
9	>100	>100	>100	65.0	3.3	>100	>100
10	>100	20.1	2.0	47.9	>100	>100	>100

Synthetic route to compounds 4–10 .Docking binding energies against cancer cell lines

Agradecimentos/Acknowledgments

UFF

Use of the vortex as a mechanochemical strategy for the synthesis of chrysin derivatives nitrated at the C6 and C8 positions of ring A

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Palavras Chave:*Nitration,vortex,flavonoids,mechanochemistry*

Highlights

Vortex mixing enabled the solvent-free, mechanochemical nitration of chrysin, achieving regioselective functionality at C6 and C8 with green nitrating systems and moderate yields.

Resumo/Abstract

Chrysin is a flavonoid widely recognized for its antioxidant, antimutagenic, and anticancer activities. Structural modification of chrysin can expand its pharmacological potential and allow further investigation of its chemical reactivity. In this context, the search for sustainable methodologies becomes essential, aligning with the principles of green chemistry, particularly the development of solvent-free reactions.[1,2]In this work, we describe an innovative method based on the use of a vortex mixer capable of promoting the automated grinding of solid samples, representing an efficient and environmentally friendly alternative to conventional mechanochemical techniques.[3]Two distinct methods were employed to obtain nitrated chrysin derivatives at the C6 and C8 positions using different nitrating agents.[4] Both methods were carried out under solvent-free conditions, in accordance with green chemistry principles, using a vortex mixer operating at 3800 rpm and 0.5 mmol scale of chrysin, employing 1 equivalent of the nitrating agent. A Falcon tube containing four stainless steel balls (5 mm) was used under agitation for 10 h, promoting efficient grinding of the solid reagents. Under these conditions, 6-nitrochrysin (15%) and 8-nitrochrysin (10%) were isolated. ^{1}H and ^{13}C NMR spectra confirmed nitration at the proposed positions, showing chemical shifts consistent with literature data (Figure 1).[5,6] This approach demonstrates that the use of a vortex mixer constitutes a simple, reproducible, and sustainable alternative for mechanochemical reactions.

Lopes, R. M.*et al.*Flavonoids.***Biotecnol. ciênc. desenvolv.***2010,*3*(14). Ma, H.*et al.***Chem. Commun.***2012,*48*(31), 3954–3956. Reynes, J. F.*et al.***ACS Org. Inorg. Au.***2024,*4*, 432–470. Barbosa, J. R. C.*et al.***JOC.***2024,*89*, 1120–1126. Zheng, Y.*et al.***Org. Lett***.2024,*26*, 3316–3320. Gurung, S. K.*et al.***Arch. Pharm. Res.***2009,*32*, 1503–1508.

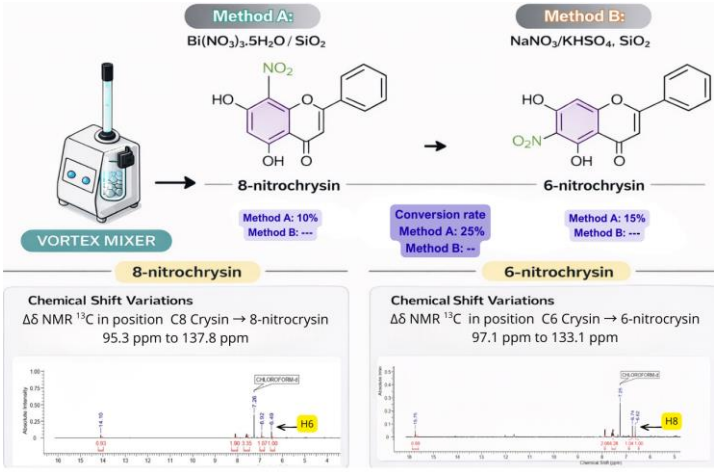


Diagram of Methods A and B showing distinct nitration patterns and chemical shift changes at C6/C8.

Agradecimentos/Acknowledgments

CAPES, CNPq, FAPESB, CIEnAm, LabSint, UFBA e UESB.

Visible-Light-Driven Synthesis of Selenium-Functionalized Juglone Derivatives through a Sustainable Approach

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Palavras Chave:*naphthoquinones,blue LED.,organochalcogen,green strategy*

Highlights

A novel blue-LED-assisted strategy enables unprecedented selective cyclization and selenium functionalization of juglones, providing selenium-rich derivatives in up to 94% yield.

Resumo/Abstract

Juglones are bioactive naphthoquinones recognized for their redox properties and ability to generate reactive oxygen species (ROS) [1]. In parallel, compounds containing chalcogens, especially selenium, stand out for modulating electronic, redox, and photophysical properties, which enhances relevant biological activities, such as antioxidant and anticancer action [2]. In this context, the present study discloses an unprecedented visible-light-assisted methodology enabling the selective cyclization and selenium functionalization of juglone derivatives under sustainable conditions. The methodology was developed from the**1**,[3] derivative of juglone, with optimization of the reaction conditions using diphenyl diselenide**2a**as a model substrate. Under irradiation with blue LED (50 W, 12 h) in the presence of $SnCl_2 \cdot 2H_2O$ (200 mol%) and CH_2Cl_2, yields of up to 85% were obtained (Table 1). The optimized conditions were then applied to a series of diaryl diselenides, resulting in compounds**3a–h**with excellent yields ranging from 29% to 94%. This photoactivated methodology stands out for its simplicity, sustainability, and high selectivity, making it a versatile and promising strategy for the functionalization of naphthoquinones with chalcogens. Currently, new structural variations are underway, including other chalcogens and different naphthoquinone cores, with the aim of expanding the scope and biological applications of these hybrids.

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Table 1. Optimization of selenocyclization reaction parameters and scope of desired compounds.

#	Visible Light (W)	Additive (mol%)	Yield (%)[a]
1	Blue LED (50)	-	18
2	Green LED (50)	-	5
3	White LED (50)	-	traces
4	Blue LED (100)	-	48
5	Blue LED (150)	-	35
6[b]	Blue LED (100)	-	46
7	Blue LED (100)	Eosin Y (5)	35
8	Blue LED (100)	CuI (10)	26
9	Blue LED (100)	$InCl_3$ (200)	45
10	Blue LED (100)	$SnCl_4$ (200)	traces
11	Blue LED (100)	$SnCl_2.H_2O$ (200)	45
12	**Blue LED (50)**	**$SnCl_2.H_2O$ (200)**	**85**
13	Blue LED (50)	$SnCl_2.H_2O$ (100)	55
14	Blue LED (50)	$SnCl_2.H_2O$ (300)	60
15	Dark	$SnCl_2.H_2O$ (200)	27

[a]Isolated yield; [b]Reaction under inert atmosphere (N_2).

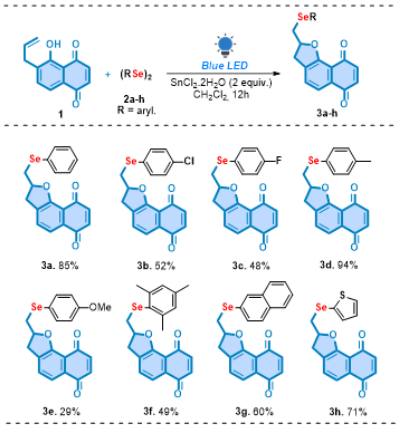


Table 1. Optimization of selenocyclization reaction parameters and scope of desired compounds.

Agradecimentos/Acknowledgments

UFF, CAPES, FAPERJ e CNPq.

Visible-Light-Promoted Iodocyclization of Juglone toward Organoselenium Hybrids

Rafael Alan Carvalho Souza (IC)*[1], Isabelly de Oliveira Ferreira (IC)[2], Luana da Silva Gomes (PQ)[3], Thaís Barreto Santos (PQ)[2], David Rodrigues da Rocha (PQ)[2], Vanessa do Nascimento (PQ)[2].

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Palavras Chave:*Photocatalysis, Naphthoquinones, Juglone.,Photocatalysis,Naphthoquinones,Juglone*

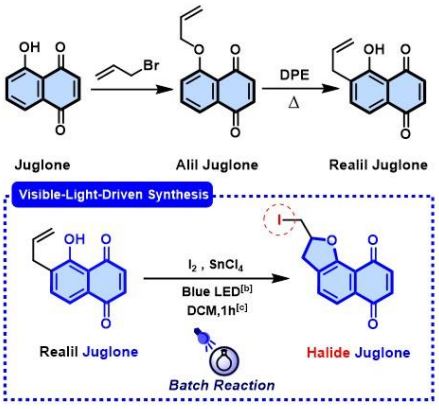
Highlights

Sustainablefunctionalization of juglone via visible-light-driven photocatalytic iodocyclization, affording a versatile iodinated naphthoquinone intermediate for incoporation of organoselenium hybrids

Resumo/Abstract

Natural naphthoquinones are emerging as privileged templates in pharmacological research due to their broad structural versatility and significant biological potential. In this context, we have developed a sustainable and innovative strategy for the functionalization of juglone. A photocatalytic iodocyclization route was systematically optimized by screening light sources, solvents, and additives, identifying the best conditions as blue light (50 W), $SnCl_4$ (200 mol%), and DCM, which afforded the iodinated intermediate in 94% yield within 1 hour. This key precursor enables the construction of triazole bridges for subsequent connection to organoselenium cores, paving the way for novel molecular hybrids with potential activity against neglected diseases such as sporotrichosis. Future work will focus on modifying the quinone core, testing alternative halogen sources, and further functionalizing this versatile intermediate through triazole-based conjugation.

#	Light Source (W)	Additive (mol%)	Solvent	Yield (%)[a]
1	Blue LED (50)	--	DCM	48%
2	Green LED (50)	--	DCM	19%
3	White LED (50)	--	DCM	39%
4	Blue LED (100)	--	DCM	20%
5	Blue LED (150)	--	DCM	15%
6	Blue LED (50)	--	Acetone	--
7	Blue LED (50)	--	THF	36%
8	Blue LED (50)	--	Toluene	28%
9	Blue LED (50)	--	EtOH	--
10	Blue LED (50)	$InCl_3$ (200)	DCM	19%
11	Blue LED (50)	Eosina Y (5)	DCM	28%
12	Blue LED (50)	$SnCl_4$ (100)	DCM	48%
13	**Blue LED (50)**	**$SnCl_4$ (200)**	**DCM**	**94%**
14	Dark	$SnCl_4$ (200)	DCM	traces



[a] Isolated by flash chromatography. [b] Chip LED (440 nm, 50 W), room temperature; [c] Reaction monitored by TLC.

Scheme 1. Synthetic route of halide juglone via photocatalysis in batch reactor.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge financial support from Brazilian Academy of Sciences (ABC), São Paulo Research Foundation (FAPESP;Grant N.: RACS, 2025/24025-0), CNPq and CAPES.

White Light–Driven Green Pathways to 2 Chalcogenonaphthalenes

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[1]Universidade Federal Fluminense; [2]Universidade Federal do Rio Grande do Sul; [3]Universidade Federal de Santa Maria

Palavras Chave:*Visible-Light,Organochalcogen,Cyclization,Photoirradiation*

Highlights

This study introduces an innovative methodology for the synthesis of 2-chalcogenonaphthalenes using visible light. Optimization studies, reaction scope expansion, and showed great results.

Resumo/Abstract

Organochalcogen compounds are valued for their structural diversity, biological activity, and redox properties, underscoring the need for obtaining this type of molecules.[1–2] In this context, several methods exist to introduce chalcogen units into organic frameworks, but most classical approaches depend on harsh conditions, such as toxic reagents, transition metals, high temperatures, and long reaction times, which limit selectivity, safety, and sustainability.[3] Thus, the development of more sustainable approaches that address current needs becomes essential, with white light standing out in this regard as a green energy source for organic reactions.[4] This research aims to establish a sustainable synthetic route for chalcogen-functionalized aromatic cores, focusing on 2-naphthalene, a compound of industrial and medicinal relevance but still underexplored due to reliance on toxic and poorly selective methods. The optimization of the reaction conditions was initially carried out using compound**1a**as the model substrate (Figure 1A). Key parameters were systematically evaluated to maximize efficiency, as summarized in Figure 1B. During this process, we varied the type of light (**entries 1–3**), the use of photocatalyst (**entries 4–6**), the reaction time and power intensity (**entries 7–9**), as well as the additive employed (**entries 10–12**). Ultimately,**condition 9**proved to be the most efficient, involving irradiation with 100 W white light for 10 hours at room temperature, using $SnCl_2.2H_2O$ as the additive. With this approach, we were able to explore a reaction scope of 15 distinct molecules, varying the dichalcogenide portion and also testing one of the compounds reactivity in subsequent reactions.

1. Organochalcogen Compounds: Elsevier, 2022.

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3. Molecules 2025, 30 (7), 1408.

4. The Royal Society of Chemistry, 2023; pp 300–333

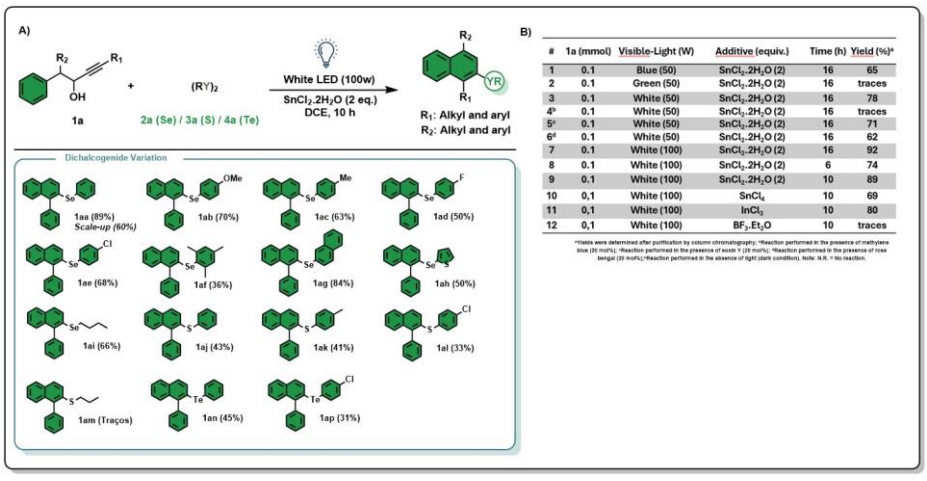


Figura 1. A) Rota sintética dos 2-calcogenonaftalenos; B) Tabela de Otimização de condições

Agradecimentos/Acknowledgments

UFF; CAPES; CNPQ; FAPERJ

49ª RASBQ
Reunião Anual da Sociedade Brasileira de Química

QPN - Produtos Naturais

Amidation of Diterpenic Acids toward New Semisynthetic Derivatives with Antileishmanial Potential

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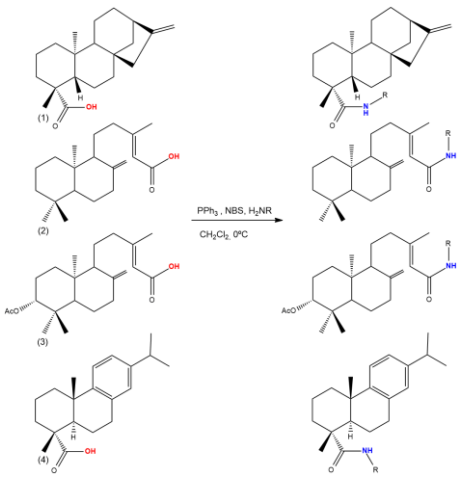
Palavras Chave:*Diterpenes,Natural products,Amidation,Leishmania amazonensis*

Highlights

Research is currently being conducted on the amidation of diterpenic acids to generate semisynthetic natural product derivatives, which will be evaluated against*Leishmania amazonensis.*

Resumo/Abstract

Natural products comprise a wide diversity of classes of chemical substances, among which diterpenes stand out, with more than 18,000 compounds already isolated[1]. These metabolites exhibit several pharmacological effects, such as antiparasitic[2], anti-inflammatory[3], and anticancer[4] activities, widely reported in the literature.The present study focuses on the isolation of diterpene acids from natural sources such as*Mikania glomerata*, copaifera oleoresin, and*Pinus Elliottii*resin. It also aims to create new semisynthetic diterpene derivatives by amidation of kaurenic, copalic, acetoxy-copalic, and dehydroabietic acids. Furthermore, the study will assess their effectiveness against*Leishmania amazonensis*.The amidation reactions between diterpenic acids and different amines were conducted following established procedures in the literature[5], using triphenylphosphine and N-bromosuccinimide in dichloromethane, with reaction progress monitored by thin-layer chromatography.Preliminary results indicate that the amidation reaction between kaurenoic acid and imidazole proceeded successfully. Structural identification of the obtained derivative was performed by ^{1}H NMR spectroscopy. The next steps involve the synthesis of the remaining derivatives, their isolation and characterization, and the evaluation of their activity against*L. amazonensis*.
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Amidation of kaurenoic (1), copalic (2), acetoxy-copalic (3), and dehydroabietic acids (4).

Agradecimentos/Acknowledgments

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An Endophytic Fungal Co-culture as a Source of 3-O-Methylfunicone Active Against Phytophthora palmivora

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Palavras Chave:*Endophytic fungi,Phytophthora palmivora,Dereplication,3-O-methylfunicone*

Highlights

A metabolomics-guided dereplication approach enabled the isolation of 3-*O*-methylfunicone from an endophytic fungal co-culture, revealing its inhibitory activity against*Phytophthora palmivora*

Resumo/Abstract

Endophytic fungi are microorganisms that colonize plant tissues without causing apparent damage to their hosts and produce specialized metabolites that enhance plant defense against pathogens and environmental stresses. In nature, these endophytes compete with other microorganisms for limited resources; however, under laboratory conditions, the biosynthesis of such metabolites is often reduced. Co-culture has emerged as an effective strategy to activate silent biosynthetic pathways by mimicking natural competitive interactions, thereby increasing chemical diversity and the production of bioactive compounds.Based on the hypothesis that resource competition between two endophytes stimulates natural products biosynthesis as a defensive mechanism, this study investigated the co-culture of*Aspergillus pseudonomiae*J1 and T*alaromyces pinophilus*J6, both isolated as endophytes from*Euphorbia umbellata.*Ethyl acetate extracts from mono- and co-cultures were analyzed by UHPLC-HRMS, and their chemical profiles were compared. A dereplication workflow was applied using MS-DIAL 4.0 software, and main metabolites were putatively identified with the aid of the SIRIUS 5 platform.The analyses revealed the presence of several natural products, including quinones, phenylpropanoids, iridoids, and funicone-type compounds. Guided by the metabolomic profile, 3-*O*-methylfunicone was isolated and structurally characterized. Bioassays demonstrated its antifungal activity against*Phytophthora palmivora*(oomycete that affects economically important food crops such as cocoa, coconut, and papaya), inhibiting mycelial growth by 54.9 ± 6.1, 30.9 ± 5.1, and 15.6 ± 6.2% at concentrations of 1.0, 0.5, and 0.25 mM, respectively. These results highlight co-culture combined with metabolomics and dereplication as a promising strategy for discovering natural products with potential anti-phytopathogenic applications.

Antagonistic Activity of Bacillus velezensis PN2-45 against Fusariosis and Metabolic Responses of Piper nigrum

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Palavras Chave:*PGPR, biocontrol, black pepper, VOCs.,PGPR,biocontrol,black pepper,VOCs*

Highlights

PN2-45 modulates VOCs, phenolics, and LOX–PAL activities, enhancing plant defense during*Fusarium*infection.

Resumo/Abstract

*Piper nigrum*is a spice of high economic value with extensive global production. However, its productivity is severely affected by fusariosis caused by*Fusarium solani*f. sp.*piperis*. This study evaluated the antagonistic activity of*Bacillus velezensis*PN2-45 and its effects on the metabolism of*P. nigrum*. In co-culture, the strain inhibited pathogen growth by 63% and by 32.98% in the sealed plate test. After that,*P. nigrum*plants were coinoculated with*B. velezensis*PN2-45 and*F. solani*f. sp.*piperis*under greenhouse conditions, with sampling at 3 and 9 weeks. Co-inoculation reduced fusariosis symptoms, whereas pathogen infection caused severe necrosis and intense defoliation. Volatile organic compounds (VOCs) were extracted by simultaneous distillation–extraction and analyzed by GC–MS. In leaves, the major VOCs were bicyclogermacrene, γ-cadinene, and α-muurolol, while roots were dominated by camphene, δ-elemene, and β-caryophyllene. Pathogen infection increased leaf α-muurolol (33.6–53%) and γ-cadinene (11.4–14.3%) contents at 3 weeks, whereas inoculation with PN2-45 increased bicyclogermacrene levels (12.5–21.39%). No significant changes in root VOC contents were observed among treatments. Leaf and root extracts were obtained by methanolic percolation, and total phenolic content (TPC) was determined by the Folin–Ciocalteu method. Co-inoculation reduced leaf TPC but significantly increased root TPC, ranging from 16.88–20.77 mg GAE g^{-1} at 3 weeks and from 20.84–25.49 mg GAE g^{-1} at 9 weeks. Lipoxygenase (LOX) activity increased in leaves of co-inoculated seedlings (7.20–8.14 × 10^{-4} M s^{-1}) at 3 weeks. Pathogen infection reduced phenylalanine ammonia-lyase (PAL) activity at 3 weeks (54–38.6 U mL^{-1}), while PN2-45 inoculation increased PAL activity at 9 weeks (54.5–72.69 U mL^{-1}). These results demonstrate the agronomic potential of*B. velezensis*PN2-45 in inducing resistance and modulating*P. nigrum*metabolism during pathogen infection.

Agradecimentos/Acknowledgments

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Antioxidant and antiglycation evaluation of the rhizome of Cyperus rotundus L.

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Palavras Chave:*Bioactive compounds,Glycation,Cyperus rotundus*

Highlights

The acetone extract of the*Cyperus rotundus*rhizome, a weed species, showed high in vitro antioxidant and antiglycation activity, with phytotherapeutic potential and alignment with SDGs 3 and 12

Resumo/Abstract

*Cyperus rotundus*L., commonly known as nutgrass (“tiririca”), is a plant belonging to the Cyperaceae family, native to tropical regions of Africa and widely distributed in tropical and subtropical areas, including Brazil [1]. It is considered one of the major agricultural weeds due to its rapid propagation through rhizomes and tubers [2]. The rhizome contains phenolic acids as its major compounds, in addition to flavonoids such as quercetin [3]. Therefore, the aim of this study was to evaluate the chemical characterization and the antioxidant and antiglycation activities of the acetone extract of*C. rotundus*rhizome.

The total phenolic content was determined using the Folin–Ciocalteu method, revealing that the rhizome has a high phenolic content, with 5649.3 ± 39.3 mg GAE/g of dry extract. Antioxidant activity was initially assessed by the DPPH● radical scavenging assay, in which the extract exhibited an IC_{50} value of 7.63 ± 0.08 µg/mL, indicating high antioxidant activity when compared with literature data. Subsequently, the reducing power was determined by the FRAP assay, showing an IC_{50} of 586 ± 15.9 at a concentration of 10 µg/mL. Finally, in the BSA/GF system, the extract demonstrated a significant capacity to inhibit the formation of advanced glycation end products (AGEs).

The results indicate that the*C. rotundus*rhizome extract exhibited strong antioxidant and antiglycation activities, suggesting potential against diabetes and diseases associated with oxidative stress. Thus, this work contributes to SDGs 3 and 12 by promoting health and well-being and encouraging responsible consumption practices through the reuse of agro-industrial residues.

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Antiparasitic Potential of Eremanthus erythropappus DC. MacLeish (Asteraceae) and compounds: In vitro and In vivo efficacy against Schistosoma mansoni

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Palavras Chave:*Eremanthus erythropappus,Schistosoma mansoni,Fridelin,Betulinic acid,Acacetin*

Highlights

LEE was more potent than EEE. Acacetin and betulinic acid were newly isolated from candeia, where only the latter had in vitro effects at*S. mansoni*. LEE and betulinic acid showed in vivo properties.

Resumo/Abstract

Schistosomiasis is a neglected tropical disease responsible for over 300,000 deaths worldwide and remains one of the most significant helminthiasis[1]. Anthelmintic chemotherapy has relied exclusively on praziquantel (PZQ) since the 1970s, contributing to risen concerns about drug resistance and increased challenge for disease control[1]. Among Brazilian folk medicine species,*Eremanthus erythropappus*, known as “candeia”, presents reported activity towards*Schistosoma*, motivating the investigation of its chemical profile and antiparasitic potential[2]. Therefore, this study evaluated the antischistosomal activity of*E. erythropappus*extracts and their metabolites against adult*S. mansoni*. In vitro assays showed that the rinsed extract (LEE) was notably more potent (EC_{50} = 18.1 µg/mL) than the ethanolic extract (EEE; EC_{50} = 191.5 µg/mL), with no cytotoxicity observed up to 500 µg/mL. UHPLC-ESI-MS/MS analysis allowed annotating 16 compounds, including sesquiterpene lactones and pentacyclic triterpenoids as a distinguishable set of metabolites among the extracts. Fractionation of LEE yielded friedelin, betulinic acid, and acacetin, with the latter two reported for the first time in*E. erythropappus*. Among the isolated compounds, only betulinic acid showed in vitro activity (EC_{50} = 36.8 µM; SI > 15.5). In vivo studies in*S. mansoni*-infected mice demonstrated that betulinic acid (400 mg/kg, oral) reduced worm burden by 41.9%, while LEE at the same dose markedly reduced worm burden (~86%), egg burden (~81%), and immature egg deposition (~87%). These findings support candeia as a promising source of antischistosomal agents.

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Antiproliferative potential of alkaloids from Tabernaemontana hystrix and T. laeta against human cervical cancer (HeLa)

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Palavras Chave:*Apocynaceae,alcaloides monoterpênicos indólicos,câncer cervical,HeLa,NIH-3T3*

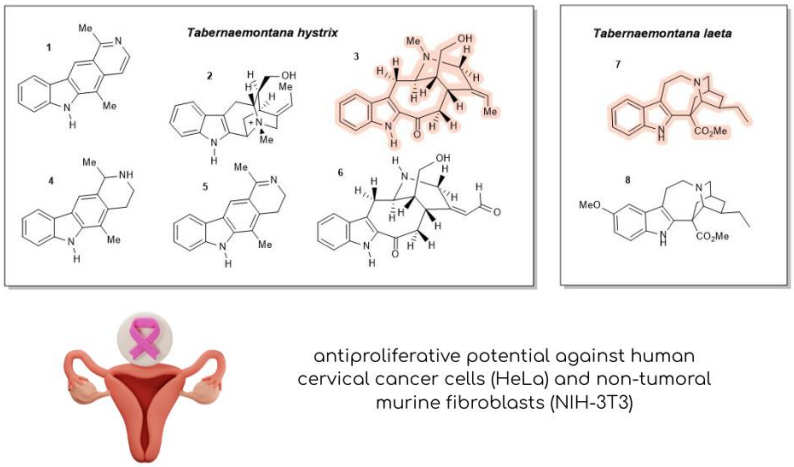
Highlights

Two monoterpene indole alkaloids showed better results than the positive control carboplatin.

*Tabernaemontana*genus is a promising source of anticancer compounds.

Resumo/Abstract

Cervical cancer is the third most incident type of cancer in the Brazilian female population. Since cancer is a public health problem in Brazil and worldwide and current drugs may present side effects or cases of multidrug resistance, the search for compounds with anticancer potential is important.*Tabernaemontana hystrix*and*T. laeta*(Apocynaceae) are native and endemic species of Brazil and are known to produce monoterpene indole alkaloids. This study aimed to evaluate the antiproliferative potential of compounds isolated from both species against human cervical cancer cells (HeLa) and non-tumoral murine fibroblasts (NIH-3T3). The alkaloids olivacine (**1**; 20.4 mg), macusine B (**2**; 131.7 mg), affinine (**3**; 391.6 mg), and a mixture (5.4 mg) of**1**(2.41%), janetine (**4**; 52.17%), and 3,14-dihydro-olivacine (**5**; 45.41%) were obtained from the EtOAc fraction of the MeOH extract of*T. hystrix*root bark. From the BuOH fraction, alkaloids**4**(18 mg) and Nb-demethyl-18-formyl-5,16-epiaffinine (**6**; 3.4 mg) were obtained, in addition to compound**1**(104.6 mg) as a precipitate. From the MeOH extract of*T. laeta*root bark, coronaridine (**7**; 32.5 mg) and voacangine (**8**; 27.8 mg) were obtained. Compounds**1**(IC_{50}/HeLa = 0.80 µg/mL; SI = 0.66),**2**(IC_{50}/HeLa > 250 µg/mL; SI = ND),**2a**(acetylated derivative of**2**; IC_{50}/HeLa > 250 µg/mL; SI = ND),**3**(IC_{50}/HeLa = 21.4 µg/mL; SI = 2.42),**4**(IC_{50}/HeLa = 26.6 µg/mL; SI = 0.73),**7**(IC_{50}/HeLa = 32.0 µg/mL; SI = 2.20), and**8**(IC_{50}/HeLa = 18.8 µg/mL; SI = 1.54) were evaluated and compared with carboplatin (IC_{50}/HeLa = 35.3 µg/mL; SI = 0.97) and doxorubicin (IC_{50}/HeLa = 0.78 µg/mL; SI = 1.28). Compounds**3**,**4**,**7**, and**8**showed better antiproliferative potential than carboplatin; however, only**3**and**7**were selective. These results highlight the potential of the genus for the discovery of anticancer compounds. Eight compounds were isolated; compounds**4**,**5**, and**6**are reported for the first time in*T. hystrix*, and compound**6**is new to the literature.



Chemical structures of monoterpene indole alkaloids isolated from T. hystrix and T. laeta

Agradecimentos/Acknowledgments

UENF, CAPES, CNPq, FAPERJ

Assessing the herbicidal activity of Caryocar Brasiliense's peel extract for sustainable and environmentally friendly weed management

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Palavras Chave:*Bioherbicide,Weed management,Caryocar Brasiliense,Germination tests,Allelopathy*

Highlights

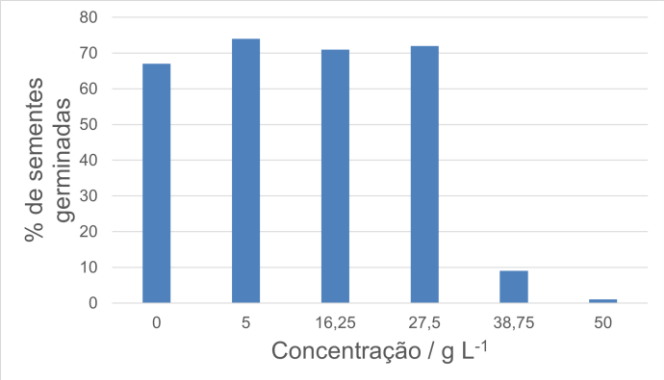
Exploring the allelopathic properties of Pequi's peel extract to discover a new possible bioherbicide for weed management. Germination tests on various plants show a positive herbicide effect.

Resumo/Abstract

The agricultural industry faces three major problems, the inadequate and excessive use of synthetic herbicides, the management of weeds and the agrifood waste. Given the extensively studied biopotential of*Caryocar Brasiliense*, the present work explores the herbicidal activity of the ethanolic extract of the Pequi peel through germination tests of various plants, including five weeds (*Euphorbia hirta, Bidens pilosa, Amaranthus retroflexus, Aeschynonmene sensitive e Commelina benghalensis*) and five economic crops (to test selectivity),*Solanum lycopersicum, Oryza sativa, Phaseolus vulgaris, Glycine max e Lactuca sativa.*

The germination tests were realized inside a seed germination chamber with a 12 h photoperiod. HS/GC-MS and LC-ESI-QToF-MS/MS analysis were carried out for the pequi peel in natura and the ethanolic fruit extract, respectively.

The germination tests suggested that the extract does present a positive herbicidal effect. The percentage of germinated seeds of*E. hirta, B. pilosa, A. retroflexus, A. sensitive*were significantly affected with the introduction of the extract. In addition to this,*E. hirta, B. pilosa, A. retroflexus*had their growths inhibited by the fruit extract. The germination tests of*S. lycopersicum*and*O. sativa*had both their germination and growth negatively affected by the extract, while the other three crops remained unaffected. While GC-MS data showed mainly aldehydes and esters in the composition of the fruit peel in natura, LC-MS data showed both gallic acid and quinic acid in the composition of the fruit extract. Both are widely reported in the literature as potent antioxidants and presenting some levels of phytotoxicity.
In conclusion, pequi's peel shows great promise as a possible bioherbicide, serving as an alternative to commercial herbicides, for the management of some of the most common weeds found in Brazil's agriculture, while also bringing more value to a commonly discarded part of the fruit.



Percentual de germinação das sementes de Amaranthus retroflexus para cada concentração do extrato.

Agradecimentos/Acknowledgments

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Avaliação do efeito da salinidade em bactérias associadas aos corais do Atlântico sul.

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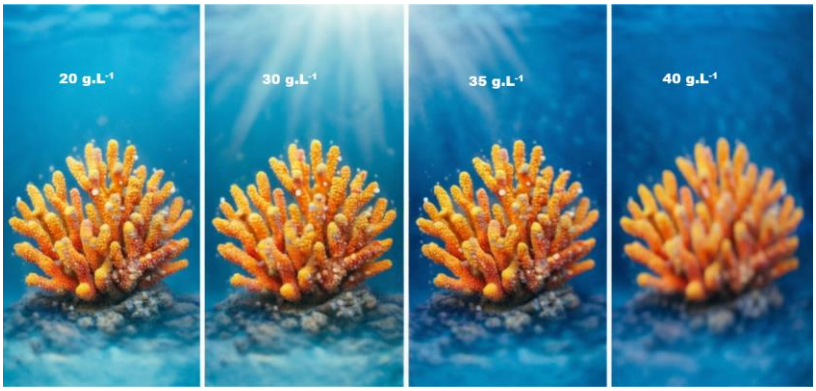
Palavras Chave:*Branqueamento, Metabolômica, Metabólitos especializados.,Global Warming,Bleaching,Metabolomics,Specialized Metabolites*

Highlights

Metabólitos microbianos que são modulados pela variação da salinidade do meio.

Resumo/Abstract

Os recifes de corais são ecossistemas altamente biodiversos, beneficiando a pesca, proteção costeira e conservação de espécies via desova. As mudanças climáticas e o aquecimento global têm causado branqueamento de corais em massa no mundo todo, incluindo no Brasil. Compreender como eles se comportam é importante para conduzir sua conservação. E para essa compreensão, o estudo da microbioma dos corais é importante pois está envolvido em vários processos químicos e biológicos. Além da variação de temperatura e pH, outros fatores como variação de salinidade também podem causar estresse nos corais e, consequentemente, o branqueamento. A salinidade do mar pode variar de acordo com o local do oceano. Por exemplo, a costa marinha próximo do estado de São Paulo, a salinidade é próxima de 35g.L -1 . Portanto, neste trabalho foi avaliado o efeito da salinidade no cultivo de diferentes bactérias isoladas do coral Mussismilia hispida coletada em São Sebastião - SP. O efeito da salinidade foi avaliado no crescimento, assim como, na produção de metabólitos pelas bactérias isoladas de corais. Para tal, as bactérias foram cultivadas em meio líquido A1 e mantidos a 25 ºC, sob agitação (200 rpm). O meio de cultivo foi preparado com água do mar artificial específico para corais nas diferentes concentrações de 20g.L -1, 30g.L -1, 35g.L -1, 40g.L -1. Os cultivos foram interrompidos com aproximadamente 8 dias, e filtrados para remoção das células. O meio líquido livre de células foi submetido à extração líquido-líquido com acetato de etila e o solvente foi evaporado sob pressão reduzida. O extrato então obtido foi analisado por cromatografia líquida acoplada espectrometria de massa e, posteriormente, esses dados foram utilizados para construção de uma rede molecular e anotação dos metabólitos no GNPS, assim, averiguando o perfil dos metabólitos produzidos nas diferentes condições investigadas.



Bactérias de coral submetidas a diferentes concentrações de salinidade

Agradecimentos/Acknowledgments

À Deus por nos dá sabedoria e ciência, à minha família, à minha orientadora professora Anelize Bauermeister, aos meus professores e à administração da Fatec Diadema e aos meus colegas de trabalho, Projeto FAPESP (processo 2024/05211-4).

Baccharis trimera Extract as a Skin-Whitening Agent for Skincare Applications

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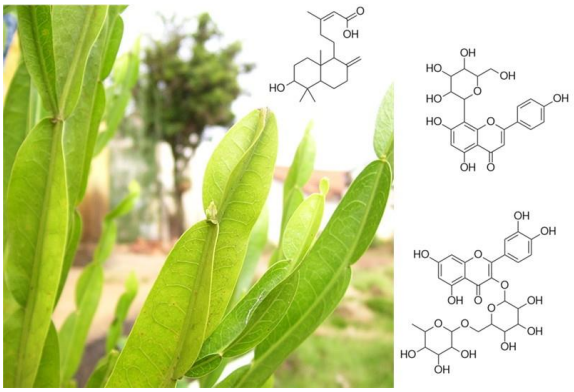
Palavras Chave:*molecular networking,Baccharis,tyrosinase,Asteraceae*

Highlights

Carqueja's skin-whitening potential: identification of a diterpene reported for the first time in this species with known anti-tyrosinase activity

Resumo/Abstract

Baccharis trimera(carqueja) is a Brazilian medicinal plant, used in phytotherapy to treat stomach disorders and widely studied for its biological potential.[1] This study evaluated the ethanolic extract of*B. trimera*for potential skincare applications, focusing on tyrosinase inhibition related to skin-whitening effects. An ethanolic extract (Sisgen A9D0265), provided by the Livealoe company, was fractionated. Tyrosinase was selected as the molecular target, and*in vitro*assays were conducted at a concentration of 100 µg/mL using L-DOPA as the substrate. Enzymatic activity was measured by spectrophotometric detection of L-dopaquinone at 475 nm.[2,3] Chemical dereplication was performed using liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) in positive ion mode. MS/MS data were analyzed using Bruker SmartFormula 3D, Compound Crawler, DataAnalysis 4.0, SIRIUS, and GNPS platform. The crude extract showed low anti-tyrosinase activity (12 ± 2% inhibition). However, fractionation significantly enhanced inhibitory effects, particularly in the dichloromethane fraction BtED (69.7 ± 3.2%) and the ethyl acetate fraction BtEA (65.3 ± 0.5%). Dereplication revealed known tyrosinase inhibitors, including rutin, apigenin flavone glucoside, and 3-hydroxy-copalic acid (Figure).[4–6]While flavonoids had been previously reported in*B. trimera*, 3-hydroxy-copalic acid, a labdane-type diterpene, was identified for the first time in this species, along with the demonstration of carqueja's skin-whitening potential.**References: 1.**Fitoterapia Brasil, 2025.*B. trimera*. https://fitoterapiabrasil.com.br/planta-medicinal/baccharis-trimera (accessed 2025).**2.**Kanlayavattanakul, M.; et al. Industrial Crops & Products 2018.**3.**da Silva CF, et al. Food Chemistry 2025.**4.**Karaoğlan, E.S., Koca, M. IJP, 2020.**5.**Kim, J.H., Kang, N.J. Korean Journal of Food Preservation 2015.**6.**Midorikawa, K., et al. Journal of Traditional Medicines 2003.



Anti-tyrosinase compounds annotated from the carqueja extract

Agradecimentos/Acknowledgments

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Bagaço de laranja: um indutor de metabólitos e bioestimulação em Bacillus velezensis?

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Palavras Chave:*metabolômica,Bacillus velezensis,economia circular,lipopeptídeos cíclicos*

Highlights

Orange waste modulates the metabolic profile of*B. velezensis*via LC-HRMS.

Modulated extracts mitigate salt stress and maintain vigor in tomato plants.

Resumo/Abstract

Frente às mudanças climáticas, bioestimulantes microbianos como o*Bacillus velezensis*surgem como uma alternativa para aumentar a resiliência agrícola devido à sua plasticidade metabólica.[1] Como essa diversidade é regulada pela disponibilidade de nutrientes no ambiente, resíduos agroindustriais complexos, como o bagaço de laranja, emergem como ferramentas estratégicas para a reprogramação de rotas biossintéticas bacterianas.[2]

Diante deste cenário, investigamos se a utilização de resíduos cítricos como substrato seria capaz de modular o metabolismo do*B. velezensis*, potencializando a ação bioestimulante e a biossíntese de moléculas relacionadas à resiliência das plantas.

Avaliamos como o teor de bagaço de laranja (0 a 10%) e o tempo de incubação (24 a 120h) modularam o metabolismo de duas cepas de*B. velezensis*. Análises por LC-HRMS revelaram que a inclusão do bagaço no meio de cultivo modulou o perfil de metabólitos secundários, favorecendo a biossíntese de auxinas em ambas as cepas, com efeito pronunciado na 3.18. Especificamente para esta cepa, o subproduto maximizou a produção de lipopeptídeos cíclicos de alto valor biotecnológico, como plipastatina A2 e B1, iturina e bacillopeptina A, sugerindo que este subproduto estimula de forma distinta o potencial metabólico de cada cepa.

A ação bioestimulante dos extratos foi validada em ensaios de germinação com sementes de alface, tomate e cenoura. Observamos que os metabólitos modulados pelo subproduto promoveram incrementos no comprimento radicular para todas as culturas, superando os controles. Sob estresse salino, os extratos mitigaram danos deletérios, mantendo o vigor e crescimento radicular no tomate. Dessa forma, os resultados confirmam que o resíduo agroindustrial atuou como um direcionador metabólico, favorecendo compostos que conferem maior resiliência vegetal frente a adversidades abióticas.

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Bank of Molecules: One Year of an Open Science Initiative to Leverage Natural Product–Based Drug Discovery in Brazil

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Palavras Chave:*Drug discovery, Brazilian biodiversity, Bioprospection, Compound management, Metabolomics*

Highlights

Brazilian biodiversity fuels a nationwide, high-throughput drug discovery platform integrating GLP workflows, metabolomics, cellular assays, and assay-ready plates.

Resumo/Abstract

Natural products remain the primary source of new therapeutic agents. Brazil is a biodiversity hotspot, offering unexplored chemical diversity with high potential for drug discovery. Despite a strong Brazilian scientific community, greater integration is required to overcome bottlenecks in early-stage drug discovery. To address this need, we established the**Bank of Molecules**, a collaborative platform designed to integrate advanced infrastructure and expertise for pharmaceutical innovation from biodiversity. Researchers may deposit chemical samples (extracts, fractions, or pure compounds) at LNBio/CNPEM with standardized metadata for traceability. Samples are registered in a certified database, processed through automated GLP-compliant workflows and stored under inert atmosphere. All deposited samples undergo two analyses: (i) untargeted metabolomic profiling for quality control and chemical space characterization, and (ii) biological evaluation using cellular assays (HCT-116 colon cancer cells and HaCaT keratinocytes) to assess anticancer activity and cytotoxicity. Chemical and biological reports are delivered within 90 days. Collaborative developments (publications and partnerships) are stimulated and defined by mutual agreement, while sample ownership remains with the depositor. Opportunities for development can also be catalyzed through the “Inova Fito Brasil” platform, in partnership with Biominas. Approved users can access samples in assay-ready plates for medium to high-throughput screening across institutions, reducing logistical barriers, ensuring traceability, and maximizing pharmacological assessment of Brazilian biodiversity molecules. The collaboration network completes its first year with 22 collaborators representing 15 institutions across eight Brazilian states (Figure 1). The first-year report will snapshot the chemical maps of the Brazilian samples in the Bank of Molecules and a diagnosis of novelty, redundancy and chemical space coverage.



Figure 1. Bank of Molecules collaboration network January to December/2025.

Agradecimentos/Acknowledgments

LNBio/CNPEM, MCTI (FNDCT), all the contributors of the Bank of Molecules and CNPEM/LNBio (LPN, FM and LGC). For more information, please contact Banco.Moleculas@lnbio.cnpem.br.

Biodegradação de polímeros mediada por Trichoderma sp.: avaliação do potencial degradativo e do perfil metabólico.

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Palavras Chave:*Resíduos,Biodegradação,Fungos,Poliméricos,Metabólitos*

Highlights

Plastic pollution causes ecological concern; Biopolymers and microorganisms are a sustainable alternative; Metabolomics showed distinct profiles across culture media.

Resumo/Abstract

Anualmente, entre 19 e 23 milhões de toneladas de resíduos plásticos são despejados nos ambientes aquáticos. Devido à baixa degradabilidade, a poluição plástica é um grande problema ecológico. Diante disso, a aplicação de biopolímeros e agentes de biodegradação tem ganhado destaque. O projeto estuda o fungo filamentoso Trichoderma sp. devido à sua capacidade de biodegradar compostos orgânicos e poliméricos, além de analisar a produção de metabólitos secundários da interação fungo-polímero em três meios de cultivo. A microscopia eletrônica de varredura confirmou a interação entre o fungo e o polímero, com sinais visíveis de degradação do material. Análises por LC-HRMS detectaram 2536 íons nos extratos obtidos a partir das análises dos cultivos, sendo 1183 íons (46,67%) no meio Batata-Dextrose(BD), 1162 íons (45,83%) no meio Malte e 190 íons (7,50%) em meio Czapek (CZ). O meio BD apresentou a maior capacidade de indução da produção de íons, seguido pelo meio Malte, enquanto o CZ apresentou os menores valores. A análise de Componentes Principais mostrou a separação entre os grupos analisados (Fungo, polímero e Fungo-polímero nos distintos meios), indicando diferenças metabólicas entre eles. Um HEATMAP foi empregado para comparação dos conjuntos de dados. Foram identificados 35 íons no total, dos quais 8 foram exclusivos no meio Czapeck, enquanto os meios BD e Malte compartilharam íons. A análise no software SIRIUS permitiu a identificação de compostos pertencentes às classes de alcaloides, cumarinas, ácidos graxos, policetídeos e carboidratos. Observou-se a redução de metabólitos do polímero, como teobromina e cafeína, indicando degradação. Os resultados mostram que a interação entre Trichoderma sp. e o polímero alterou significativamente o perfil metabólico do fungo, com produção de diferentes classes de metabólitos secundários em função do meio de cultivo. Ademais, as evidências de biodegradação reforçam o promissor potencial do fungo em aplicações sustentáveis.

Biological Control of Fusariosis and Yellow Wilt in Black Pepper by Bacillus velezensis PN2-45 and Its Effects on Plant Metabolism

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Palavras Chave:*PGPR, biocontrol, black pepper, VOCs.*

Highlights

*Bacillus velezensis*PN2-45 reduces Fusarium disease symptoms under greenhouse conditions.

PN2-45 modulates VOCs, phenolics, and LOX–PAL activities, enhancing plant defense during*Fusarium*infection

Resumo/Abstract

Black pepper (*Piper nigrum*) production in Pará state faces severe limitations due to endemic pathogens such as*Fusarium oxysporum*(FO) and*F. solani*f. sp.*piperis*(FSP), the causal agents of yellow wilt and root rot. This study evaluated the biocontrol potential of*Bacillus velezensis*PN2-45, isolated from healthy rhizospheres of*P. nigrum*. In vitro, PN2-45 inhibited mycelial growth of FO (72.9%) and FSP (63.1%) by in dual culture assay, while its crude extract (10 mg/mL) reduced growth by 39.93% and 56.32%, respectively. GC-MS analysis identified antifungal VOCs such as dodecanal, n-decanal, 2-ethyl-hexanol, and 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-3-buten-2-one. LC-MS/MS analysis revealed bacillibactin and surfactins (C12–C16) as major metabolites, along with minor compounds annotated via GNPS2. To verify in vivo efficacy,*P. nigrum*plants were coinoculated with PN2-45 and both pathogens separately, with sampling at 3 and 9 weeks. In vivo assays demonstrated that co-inoculation with PN2-45 reduced disease severity compared to pathogen-only treatments, which showed necrosis and defoliation. VOC profiling indicated that infection altered leaf and root chemical composition, with sesquiterpenes such as α-muurolol, γ-cadinene, bicyclogermacrene, and β-caryophyllene predominating. PN2-45 modulated these profiles by increasing bicyclogermacrene in leaves and reducing β-caryophyllene in roots, suggesting interference in pathogen-associated metabolism. Biochemical analyses showed induction of plant defense responses, including increased lipoxygenase (LOX) activity and enhanced phenylalanine ammonia-lyase (PAL) activity at later stages. Co-inoculation also increased total phenolic content in roots. Overall, PN2-45 modulates plant metabolism and induces resistance mechanisms, highlighting its potential as a sustainable biocontrol agent.

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Bioprospecting in Aspidosperma spp.: Isolation, Characterization, and Evaluation of Antimycobacterial, Anti-inflammatory, and Cytotoxic Potential

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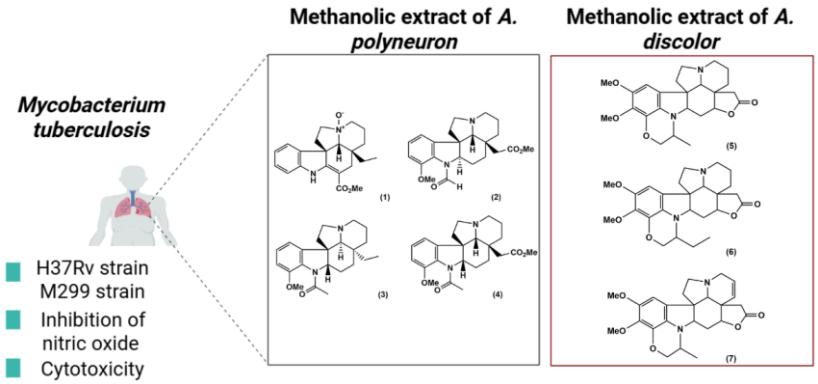
Palavras Chave:*Indole Alkaloids,Apocynaceae,Aspidosperma,Antimycobacterial Activity,Anti-inflammatory Activity*

Highlights

Phytochemical study of*A. polyneuron*and*A. discolor*seeds resulted in seven indole alkaloids. Extracts showed ant-*Mtb*activity. *A. polyneuron*reduced NO production 27 fold greater than the control.

Resumo/Abstract

Tuberculosis, a neglected disease caused by*Mycobacterium tuberculosis*(*Mtb*), affects more than 10 million people annually and accounts for approximately 1 million deaths worldwide, according to the WHO. Approximately 78% of cases are multidrug-resistant, compromising therapeutic efficacy and highlighting the need for new treatment strategies.*Aspidosperma*species produce monoterpene indole alkaloids, frequently associated with anti-inflammatory and antitumor properties. In this context, the present study aimed to isolate, identify, and evaluate the antimycobacterial, anti-inflammatory, and cytotoxic potential of methanolic seed extracts from*A. polyneuron*(**AP**) and*A. discolor*(**AD**). The**AP**and**AD**extracts exhibited antimycobacterial activity against the H37Rv strain, with MIC_{50} values of 33.74±0.04 and 80.82±0.06 µg/mL, respectively. Against the highly virulent M299 strain,**AP**maintained activity (MIC_{50}= 263.7±0.004 µg/mL), whereas**AD**showed lower efficacy (MIC_{50}> 400 µg/mL). Both extracts displayed low cytotoxicity in RAW 264.7 macrophages and high selectivity indices. Notably, the**AP**extract inhibited nitric oxide (NO) production at 0.5±0.04 µg/mL, a value substantially lower than that observed for the positive control L-NMMA (13.2±0.6 µg/mL), demonstrating pronounced anti-inflammatory potential associated with antimycobacterial activity. From the CH_2Cl_2 fraction of the**AP**extract, the alkaloids aspidospermidine (**1**), cylindrocarine (**2**), aspidospermine (**3**), and cylindrocarpidine (**4**) were isolated. From the**AD**extract, the alkaloids dihydro-obscurinervidine (**5**), dihydro-obscurinervine (**6**), and obscurinervidine (**7**) were obtained. These results highlight*Aspidosperma*species as sources of compounds with combined antimycobacterial and anti-inflammatory activities. Furthermore, the phytochemical study led to the isolation of seven compounds, five of which (**1**,**4**-**7**) are reported for the first time in these species, contributing to the chemical knowledge of the genus.



Chemical structure of alkaloids isolated from the extract of A. polyneuron and A. discolor.

Agradecimentos/Acknowledgments

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Bioprospecting of flavonoids from Chromolaena hirsuta: Molecular Networking, Structural Elucidation, and anti-Leishmania amazonensis activity

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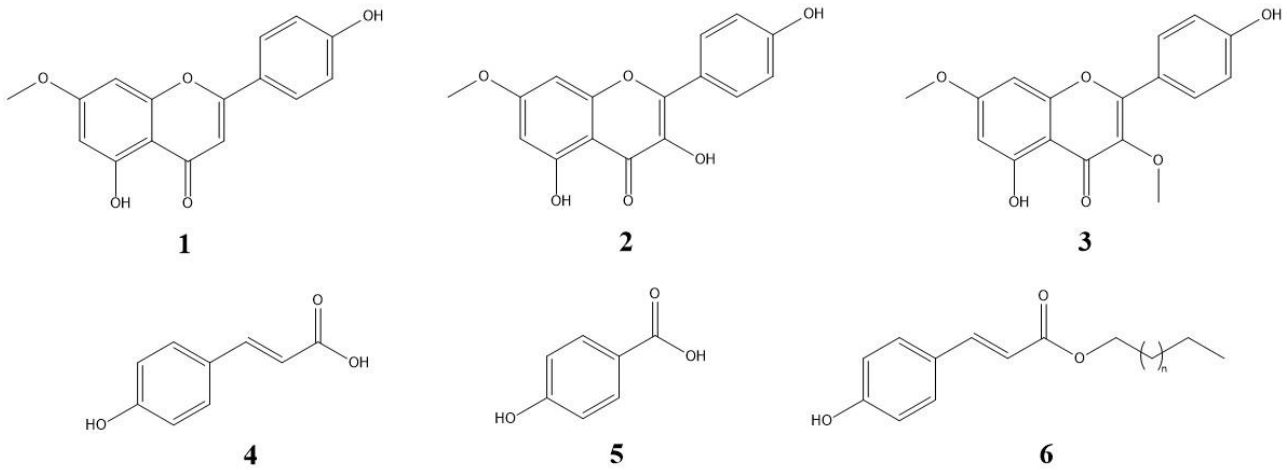
Palavras Chave:*Campos Gerais, Asteraceae, methoxylated flavonoids*

Highlights

Putative annotation of 16 flavonoids. Approximately 70% are methoxylated flavonoids. A new fatty acid ester of*p*-coumaric acid. Promising anti*Leishmania*activity with high selectivity.

Resumo/Abstract

Flavonoids are an important taxonomic marker for*Chromolaena*, as they have been reported in 20 of the 26 species investigated. Approximately 80% of the flavonoids isolated from this genus are methoxylated.[1] Our research group has previously studied three*Chromolaena*species occurring in the Campos Gerais region of Paraná, and our findings corroborate this chemotaxonomic profile.[2,3,4] This study investigated the chemical composition of the aerial parts of*C. hirsuta*, a South American native species that also occurs in the Campos Gerais. Molecular networking was employed to facilitate the flavonoids annotation in*C. hirsuta*, in combination with isolation, structural elucidation, and evaluation of anti-*Leishmania amazonensis*activity. Dereplication enabled the putative annotation of 16 flavonoids, and three were isolated and identified as genkwanin (**1**), rhamnocitrin (**2**) and kumatakenin (**3**). In addition to the flavonoids,*p*-coumaric acid (**4**),*p*-hydroxybenzoic acid (**5**), and a fatty acid ester of*p*-coumaric acid (**6**) was isolated (**Fig. 1**). The ester structure was proposed based on key HMBC correlations, including the methylene protons at δH 4.21 (t,*J*= 6.8 Hz) to the carbonyl group at δC 167.5, as well as correlations of the*trans*-olefinic protons at δH 7.63 (d,*J*= 15 Hz) and δH 6.33 (d,*J*= 15 Hz) with the same carbonyl carbon. The crude extract of*C. hirsuta*showed an IC_{50} of 9.62 ± 1.40 and a selectivity index (SI) of 21 against*L.amazonensis*amastigotes, whereas the hexane fraction showed an IC_{50} of 3.68 ± 0.05 and an SI of 19. Overall, both samples exhibited promising anti-*Leishmania* activity with high selectivity. ^{1}H NMR spectrum of the hexane fraction indicated that*p*-coumaric acid fatty acid esters are major constituents, which may be associated with the activity observed for this fraction. A total of 16 flavonoids were putatively identified most of them methoxylated (11), corroborating the known chemotaxonomic profile of the genus.



Compounds isolated from Chromolaena hirsuta

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CARACTERIZAÇÃO E QUANTIFICAÇÃO DE METABÓLITOS SECUNDÁRIOS EM VARIEDADES CRIOULAS DE INHAME/CARÁ POR CROMATOGRAFIA LÍQUIDA DE ALTA EFICIÊNCIA (HPLC)

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Palavras Chave:*Metabólitos secundários,Cará,Cromatografia líquida,Caracterização química.*

Highlights

Chemical profiling of yam landraces reveals rich flavonoid and anthocyanin diversity, highlighting their nutritional and functional potential in organic farming systems.

Resumo/Abstract

A manutenção da agrobiodiversidade, especialmente por meio da preservação de variedades crioulas, é fundamental para a sustentabilidade da agricultura orgânica, pois contribui para a resiliência dos sistemas produtivos e para a oferta de alimentos com maior valor nutricional. Nesse contexto, a caracterização química desses recursos genéticos é essencial para compreender seu potencial funcional e agregar valor às culturas tradicionais. Assim, este trabalho teve como objetivo identificar e quantificar flavonoides e antocianinas presentes em diferentes variedades de inhame e cará utilizando Cromatografia Líquida de Alta Eficiência (HPLC). A metodologia envolveu o preparo das amostras, com etapas de maceração, filtração em membranas apropriadas e análise cromatográfica em coluna C18. Para a determinação de flavonoides, utilizou-se detecção em 291 nm e fase móvel isocrática, permitindo a identificação de compostos como pinostrobina e crisina. As antocianinas foram analisadas com detecção em 518 nm, utilizando fase móvel acidificada e purificação prévia por extração em fase sólida (SPE), garantindo maior seletividade analítica. Os resultados indicaram que a pinostrobina foi o flavonoide mais abundante, presente em todas as variedades analisadas, com concentrações entre 0,733 ppm e 3,754 ppm, sendo o Cará Roxo Comprido da Mata a variedade com maior teor. A crisina foi identificada exclusivamente no Cará Ferro do Maranhão, com concentração de 2,05 ppm. Na análise das antocianinas observou-se grande variabilidade entre as amostras, destacando-se a Peonidin 3-O-Glucoside Chloride como o composto de maior concentração entre os pigmentos detectados. De modo geral, as análises cromatográficas evidenciaram diversidade no perfil de compostos bioativos entre as variedades crioulas estudadas, reforçando a importância da conservação da agrobiodiversidade e o potencial dessas culturas como fontes de compostos bioativos associados à promoção da saúde.



Extrato de antocianinas do Cará Roxo Comprido da Mata obtido para análise cromatográfica por HPLC

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Chemical annotation and biological activities of the Amazonian species Clusia grandiflora: antileishmanial and anti-inflammatory activity

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Palavras Chave:*Clusiaceae,prenylated benzophenones,HPLC-ESI-IT/MS,L. (L.) amazonensis,Cell death*

Highlights

Fruits of*C. grandiflora*are rich in prenylated benzophenones.

FDCG and FHex showed moderate antileishmanial activity against promastigotes;

The samples significantly reduced nitric oxide production.

Resumo/Abstract

The public health scenario in Brazil is marked by the occurrence of several diseases that affect the population, including neglected diseases. Leishmania infection affects approximately one million people per year worldwide. In this context, therapeutic alternatives are being sought from bioproducts derived from the Brazilian flora, such as*Clusia grandiflora*, a member of the Clusiaceae family popularly known as “orelha de onça”. The present study aimed to perform the chemical annotation of the hydroethanolic extract obtained from the fruits of*C. grandiflora*(EBCG) and its dichloromethane (FDCG) and hexane (FHex) fractions, as well as to investigate their antileishmanial and anti-inflammatory activities, mechanisms of parasite cell death, and nitric oxide (NO) production. The extract and fractions were annotated by high-performance liquid chromatography coupled with electrospray ionization ion trap mass spectrometry (HPLC–ESI–IT/MS). Chemical annotation predominantly revealed the presence of polyprenylated benzophenones. FDCG and FHex exhibited moderate antileishmanial activity against promastigote forms, with IC_{50} values of 20.34 and 85.86 µg mL^{-1}, respectively. In the amastigote forms, only FHex was active, with an IC_{50} of 7.0 µg mL^{-1}. Cell death analysis demonstrated distinct mechanisms depending on the parasite stage, with predominantly necrotic death in promastigotes and apoptotic death in amastigotes, suggesting stage-specific modes of action. Furthermore, all samples significantly reduced NO production, indicating relevant immunomodulatory and anti-inflammatory effects. Overall, the results highlight the fruits of*C. grandiflora*as a promising source of prenylated benzophenones with antileishmanial and anti-inflammatory potential.

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UFMA, LQPN, CAPES, FAPEMA, PPBio

Chemical Characterization and Larvicidal Activity of the Essential Oil and Major Constituents of Etlingera elatior var. tulipa Against Aedes aegypti

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Palavras Chave:*Essential Oil,Larvicidal,Aedes aegypti,Etlingera elatior*

Highlights

Essential oil and major constituents of*Etlingera elatior*(tulipa variety) showed larvicidal activity (LC_{50}: 13.34–126.90 µg/mL) against*Aedes aegypti*, standing out as a potential natural alternative.

Resumo/Abstract

Arboviral diseases transmitted by the vector*Aedes aegypti*are a major global public health concern each year, particularly in Brazil[1]. To prevent the spread of these diseases, an integrated set of actions is required, ranging from vaccines, which present age restrictions and low adherence, to the elimination of all stages of the mosquito's life cycle. However, the use of synthetic chemical products to control this vector may pose risks to human health and the environment, in addition to promoting the emergence of more resistant strains[2]. In this context, essential oils represent a biorenewable source of effective larvicidal compounds with lower toxicity to non-target organisms[3]. Thus, the present study aimed to analyze the chemical composition and larvicidal activity of the essential oil and its major constituents (dodecanol and dodecanal) from*Etlingera elatior*(tulipa variety) against*Aedes aegypti*. The essential oil was obtained by hydrodistillation, with a yield of 0.07%, and analyzed by gas chromatography coupled to mass spectrometry (GC/MS), which identified dodecanal (40.66%) and dodecanol (28.95%) as the major constituents. Larvicidal activity evaluated after 48 h showed an LC_{50} of 54.44 µg/mL for the essential oil, while dodecanol presented an LC_{50} of 13.34 µg/mL. Dodecanal is still under evaluation. The results demonstrate that the essential oil and its major constituents exhibit larvicidal activity, representing a promising and still underexplored natural alternative for vector control. This study is pioneering in the evaluation of the larvicidal activity of the tulip variety of*Etlingera elatior*against*Aedes aegypti*.

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Chemical complexity and stereochemical specificity of stink Bug sex pheromones.

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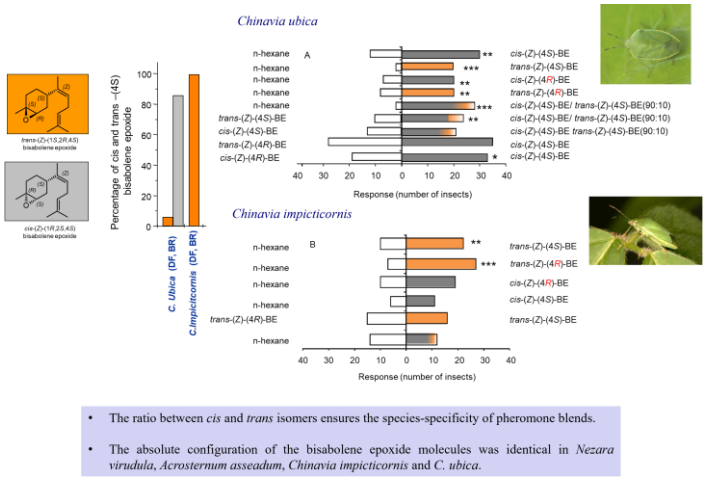
Palavras Chave:*pheromones,stereochemistry,biological activity,stink bugs*

Highlights

Stink bug sex pheromones are species-specific. This specificity relies on differences in chemical structures, pheromone components, blend ratios, and both absolute and relative stereochemistry.

Resumo/Abstract

Stink bugs rely on chemical signalling to mediate communication over long, medium, and short distances, enabling host location, mate finding, and resource exploitation. Their semiochemical comprise a diverse array of signals, including sex, aggregation, and alarm pheromones, as well as allomones, kairomones, and synomones. Several previous studies have demonstrated that stereochemistry is a key component of pheromone biological activity, influencing the in insect behavioural responses. In Pentatomidae, this complexity is exemplified by the production of different stereoisomers and component ratios of sesquiterpenes and methyl esters among species. Most species exhibit a species-specific blend of pheromone components. This specificity generally results from differences in the composition of the blend, either using distinct molecules or through variations in the relative ratios of shared compounds. For instance, rice stink bugs produce distinct stereoisomers of 1,10-bisaboladien-3-ol, while*Chinavia*spp. and*Nezara viridula*rely on specific ratios of cis- and trans-(Z)-bisabolene epoxides for species-specific communication. In the Neotropical brown stink bug*Euschistus heros*, the (2S,6R,10S)-trimethyltridecanoate isomer is highly attractive to females, whereas other stereoisomers show reduced or no activity. Despite their potential for pest monitoring and management, the chemical and behavioural complexity of stink bug pheromones has limited their broader application in agroecosystems. Here, we present microchemical approaches combined with chiral gas chromatography to elucidate the chemical structures of sex pheromones from economically important stink bug species in Brazilian arable crops, emphasizing the critical role of stereochemistry in shaping biological activity and applied potential.



Responses of Chinavia impicticornis and Chinavia ubica to stereoisomers of their sex pheromones

Agradecimentos/Acknowledgments

Funding: CNPQ,FAP-DF, INCT-NanoAgro, Embrapa

Chemical composition and antioxidant activity of the volatile and non-volatile compounds of ubaia fruit (Eugenia patrisii)

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Palavras Chave:*Flavonoids,sesquiterpenes ABTS,DPPH,GNPS2,sesquiterpenes,ABTS*

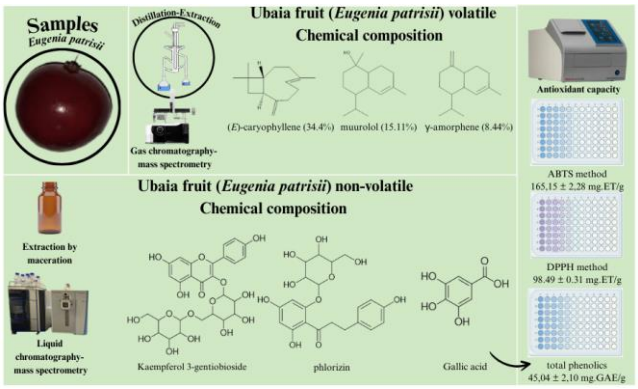
Highlights

-This is the first study to describe*Eugenia patrisii*fruits volatile concentrate (VC) and hydroethanolic extract (HEU).

- The HEU was rich in flavonoids, whereas the VC was rich in sesquiterpenes.

Resumo/Abstract

*Eugenia patrisii*Vahl (Myrtaceae) fruits are known as Ubaia or Amazonian cherry. The fruits are red-colored and consumed fresh or as a refreshing beverage [1]. This study aimed to characterize the chemical composition of the volatile concentrate (VC) and the hydroethanolic extract of the ubaia fruit pulp (HEU), as well as to evaluate the antioxidant capacity and the total phenolic content (TP). The fruits were purchased at the Ver-o-Peso open-air market (Belém, PA, Brazil). The VC was obtained by simultaneous distillation–extraction using a Nickerson and Likens apparatus, and analyzed by gas chromatography–mass spectrometry [2]. For HEU preparation, the lyophilized fruit pulp (50 g) was subjected to successive extractions with hexane and 70% ethanol. The chemical characterization of the HEU was performed by liquid chromatography coupled to Orbitrap mass spectrometry in negative ion mode, using the GNPS2 and MoNA libraries. The antioxidant capacity of the HEU was evaluated using the DPPH and ABTS assays, and the TP content was determined by the Folin–Ciocalteu method. In the VC analysis, a predominance of sesquiterpenes was observed, with mainly (*E*)-caryophyllene (34.40%), γ-amorphene (15.11%), and epi-α-muurolol (8.44%). The HEU showed a predominance of flavonoids, such as kaempferol-3-gentiobioside, phlorizin, and quercetin-O-galactoside, in addition to organic acids, such as digalloyl hexoside and gallic acid. The antioxidant capacities of HEU were 165.15 ± 2.28 mgTE/g (ABTS) and 98.49 ± 0.31 mgTE/g (DPPH). The average total phenolic content was 45.04 ± 2.10 mgGAE/g, corroborating the direct relationship between the presence of phenolic compounds and flavonoids and the observed antioxidant capacity [3]. This is the first study to describe VC and HEU. The results indicate that HEU, due to its richness in flavonoids and high antioxidant capacity, presents potential for future*in vivo*investigations, such as anti-inflammatory and oxidative stress assays.



Agradecimentos/Acknowledgments

We thank the CNPq for funding this research through the Pró-Amazônia (Call for Proposals No. 19/2024). We also thank the PADAP research group, LAQUIPRON, CMABio, and UEPA for their institutional support.

Chemical composition and antioxidant activity of volatile and non-volatile compounds of Plinia cauliflora (Mart.) Kausel

Samantha de Lima Ferreira (IC)[1], Raphael Oliveira de Figueiredo (PG)*[1], Matheus da Costa de Almeida (IC)[1], Carlos Vinícius Azevedo da Silva (PG)[2], Hector Henrique Ferreira Koolen (PQ)[2], Joyce Kelly do Rosário da Silva (PQ)[3], Pablo Luis B. Figueiredo (PQ)[1].

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Palavras Chave:*CG-EM,LC-MS/MS,ABTS,DPPH,Flavonoids*

Highlights

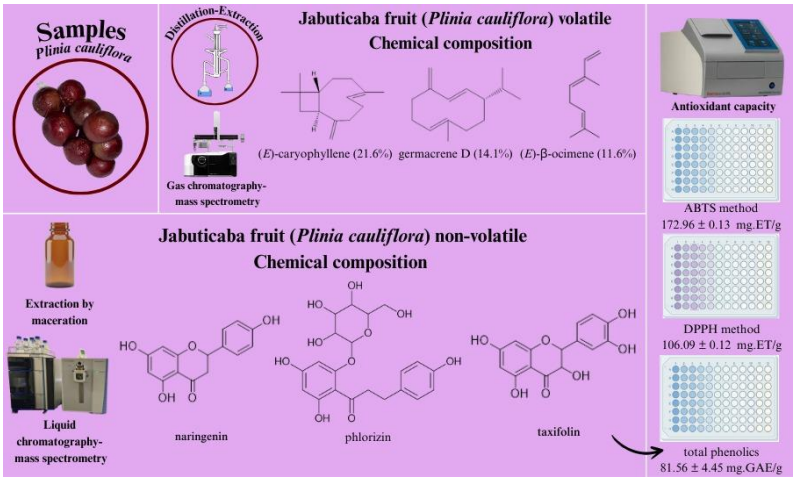
Jabuticaba pulp extracts showed high antioxidant activity in DPPH and ABTS assays

Resumo/Abstract

Plinia cauliflora(Myrtaceae)is a native species rich in bioactive compounds, especially phenolics and flavonoids, associated with potential antioxidant activity. This work has objective the characterize the chemical composition of the volatile concentrate (VC) and the hydroethanolic extract of*P. cauliflora*(EPC) from the fruit pulp, as well as to evaluate the antioxidant capacity and total phenolic content (TPC) of the extract. The plant material was acquired at the Ver-O-Peso open-air market (Belém, PA, Brazil). The VC was obtained by simultaneous distillation-extraction in a Nickerson & Likens extractor and analyzed by GC-MS. The pulp (50g) was lyophilized and subjected to sequential exhaustive removal with hexane, followed by hydroethanolic extraction (70% ethanol). The extract was concentrated in a rotary evaporator, and the antioxidant capacity was evaluated by the DPPH and ABTS methods, and the TP by Folin-Ciocalteu. The EPC chemical composition was performed by liquid chromatography was confirmed to obitrap mass spectrometry (LC-MS/MS) in negative mode, using the GNPS2 and MoNA libraries. VC showed a predominance of sesquiterpene hydrocarbons: (*E*)-caryophyllene (21.6%), germacrene D (14.1%), β-elemene (6.9%), viridiflorene (6.3%), thus classes the monoterpene hydrocarbons: (*E*)-β-ocimene (11.6%) and silvestrene (8.6%). While EPC was characterized mainly by flavonoids: naringenin, phlorizin, quercetin-O-galactoside, taxifolin 7-glucoside and kaempferol 3-gentiobioside. The antioxidant assays (DPPH, 106.09 ± 0.12 mgET/g; ABTS, 172.96 ± 0.13 mgET/g) and the TP (81.56 ± 4.45 mgEAG/g) are related to those reported in the literature, Therefore the significant antioxidant capacity of the extract.

Reference

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[2] Barros, A. S., et al (2024).*Foods*,*13*, 1490.
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Chemical composition and antioxidant activity of volatile and non-volatile compounds Plinia cauliflo

Agradecimentos/Acknowledgments

We thank CNPq for funding this research through Pró-Amazônia (Call for Proposals 19-2024). We also thank PADAP research group, LAQUIPRON, and UEPA for their institutional support.

Chemical composition of volatiles and non-volatiles of three Arecaceae fruits

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Palavras Chave:*LC-MS/MS,GC-MS,Flavonoids,Cell viability,MTT.*

Highlights

This is the first report on volatiles of*Oenocarpus bacaba*,*Attalea maripa,*and*Astrocaryum aculeatum*.

This is the first report on non-volatile of*A. maripa*.

Resumo/Abstract

The chemical characterization of Amazonian fruits has revealed a wide diversity of volatile and phenolic compounds with scientific interest. This work aims to characterize the chemical composition of the volatile concentrate (VC) and the hydroethanolic extract of*Oenocarpus bacaba*(OB),*Attalea maripa*(AM), and*Astrocaryum aculeatum*(AA). The VC was obtained by simultaneous distillation-extraction (SDE) in a Nickerson & Likens extractor and analyzed by GC-MS. To obtain the hydroethanolic extract, the pulps (50 g) were lyophilized and subjected to sequential exhaustive extraction with hexane, followed by hydroethanolic extraction. The extracts were concentrated in a rotary evaporator and analyzed by LC-MS/MS in negative mode, with comparison of the spectra to the GNPS2 and MoNA libraries. In the VC, OB showed a predominance of oxygenated sesquiterpenes, with curzerene (74.1%) being the most prominent. AM presented fatty acid derivatives, such as hexanal (17.21%), and monoterpene hydrocarbons, mainly sabinene (42.57%), limonene (10.1%), (*Z*)-β-ocimene (7.36%), and β-pinene (5.79%). In AA, methyl hexanoate (75.85%), sabinene (9.86%), and limonene (3.36%) were predominant. No reports were found in the literature on the CV of fruit pulp obtained by SDE. In the hydroethanolic extracts, flavonoids were predominantly observed, including naringenin (OB, AA and AM), catechin (OB), vicenin-2 (OB), quercetin diglycoside (OB), narcissin (AM), nicotiflorin (AA), isovitexin (OB), isorhamnetin (OB) and apigenin (OB), as shown in the molecular network generated in GNPS (Figure 1). These results agree with studies that report the recurrent presence of these flavonoids in OB and AA, while for AM there are still scarce records of these metabolites. Further studies are needed to deepen the understanding of the chemical profile of these species.

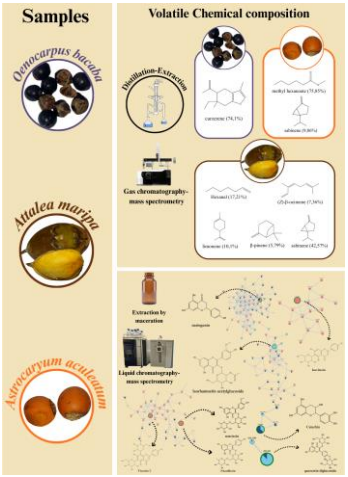


Figure 1. Chemical composition of volatiles and non-volatiles of three Arecaceae fruits

Agradecimentos/Acknowledgments

We thank CNPq for funding this research through Pró-Amazônia (Call for Proposals 19-2024). We also thank CMABio and UEPA for their institutional support.

Chemical composition, physical properties, and in vitro cytotoxicity of Hyptis crenata essential oil

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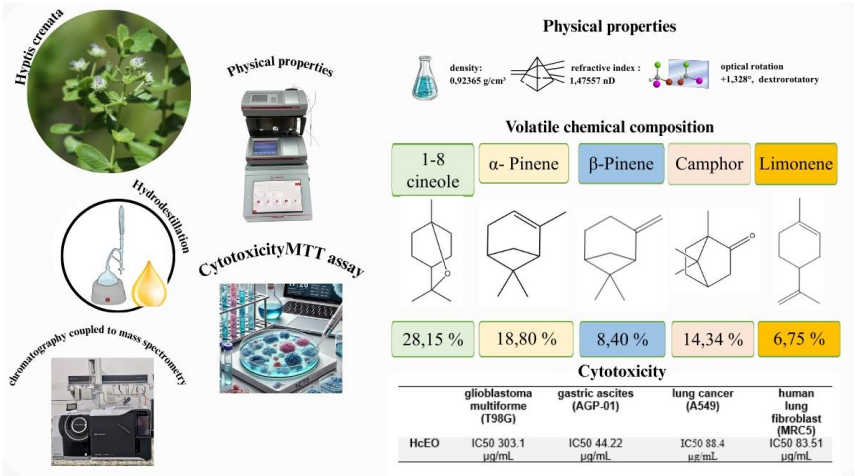
Palavras Chave:*salva-do-Marajó, Monoterpines, MTT, volatiles.*

Highlights

-*Hyptis crenata*essential oil showed moderate*in vitro*cytotoxicity.

Resumo/Abstract

*Hyptis crenata*Pohl ex Benth. (Lamiaceae), known as salva-do-marajó, is traditionally used in the treatment of inflammation and pain. This study aims to characterize the chemical composition, physical properties, and evaluate the in vitro cytotoxicity of the*H. crenata*essential oil (HcOE). The specimen was collected in the municipality of Salvaterra, Pará. HcEO was obtained by hydrodistillation. A voucher (MG-241933) was incorporated into the Herbarium of the Museu Emílio Goeldi. The collection followed the Brazilian biodiversity laws (SISGEN A090EB2). The chemical composition was analyzed by gas chromatography coupled to mass spectrometry. The physical properties were measured using an integrated Anton Paar instrument, composed of an Abbemat 300 refractometer, an MCP 100 polarimeter, and a DMA 4501 densimeter. Cytotoxicity was evaluated using the MTT assay against glioblastoma multiforme (T98G), gastric ascites (AGP-01), lung cancer (A549), and human lung fibroblast (MRC5) cell lines. The HcEO yield was 2.8%. Thus, 41 constituents were identified, comprising 92.95% of the total composition of HcEO, with a predominance of oxygenated monoterpenes (44.47%) and hydrocarbon monoterpenes (43.13%). The main constituents (>5%) were 1,8-cineole (28.15%), α-pinene (18.80%), camphor (14.34%), and β-pinene (8.40%). The HcEO had density of 0.92365 g/cm³, refractive index of 1.47557, and positive optical rotation of +1.328° at 20 °C, indicating dextrorotatory behavior and values compatible with oils predominantly composed of monoterpenes. The OEHc demonstrated cytotoxicity in all cell lines: T98G (IC50 303.1 µg/mL), AGP-01 (IC50 44.22 µg/mL), A549 (IC50 88.4 µg/mL), and MRC5 (IC50 83.51 µg/mL), indicative of predominantly moderate cytotoxic activity. These results corroborate the pharmacological potential of HcEO in antineoplastic treatment strategies.



Cytotoxicity of leaf and resin essential oils from Hyptis crenata in the Amazon Region

Agradecimentos/Acknowledgments

We thank CNPq for funding this research through Pró-Amazônia (Call for Proposals 19-2024). We also thank PADAP research group, LAQUIPRON, FAPESPA, and UEPA for their institutional support.

Chemical investigation of Dolichandra unguis-cati and antimicrobial activity.

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Palavras Chave:*Bignoniaceae,verbascoside,antimicrobial,HPLC*

Highlights

This study describes the chemical composition of the leaf extract of*D. unguis-cati*, the isolation of verbascoside, and the evaluation of the antimicrobial activity of the extracts and fractions.

Resumo/Abstract

*Dolichandra unguis-cati*or*Macfadyena unguis-cati*(Bignoniaceae) is a climbing species widely distributed in the Americas. Popularly known as “cat’s claw,” “bat’s claw,” “bat vine,” and “golden vine,” it is extensively used in traditional medicine for the treatment of hepatitis, venereal diseases, snakebites, malaria, dysentery, rheumatism, and inflammatory conditions[1]. Previous scientific studies have reported the presence of secondary metabolites such as saponins, flavonoids, triterpenes, lignans, and phenylethyl glycosides in this species[2]. Therefore, the aim of this work was to investigate the chemical composition of the leaf extract of*D. unguis-cati*, to isolate compounds from this extract, and to evaluate their antimicrobial activity. The methods employed included classical phytochemical techniques, analyses by Ultra-Performance Liquid Chromatography coupled with High-Resolution Mass Spectrometry (UPLC-HRMS/MS), and preparative HPLC. The extracts and fractions were evaluated in susceptibility assays against*Fusarium oxysporum*(sequenced environmental isolate – F4),*Staphylococcus aureus*(ATCC 25923), and*Pseudomonas aeruginosa*(clinical isolate). Among the compounds identified through molecular networking using GNPS, verbascoside (**1**) was isolated from the*n*-butanol fraction by preparative HPLC, and its chemical structure was elucidated by Nuclear Magnetic Resonance (NMR) spectroscopy. Among the samples evaluated in the biological assays, the best MIC (Minimum Inhibitory Concentration) value was 125 mg/mL, obtained for the ethyl acetate subfraction against*S. aureus*. The chemical characterization of*D. unguis-cati*enabled the identification of specialized metabolites, with emphasis on the isolation of verbascoside. The antimicrobial activity observed, particularly against*S. aureus*, reinforces the bioactive potential of this species and highlights the relevance of dereplication strategies in studies of medicinal plants.

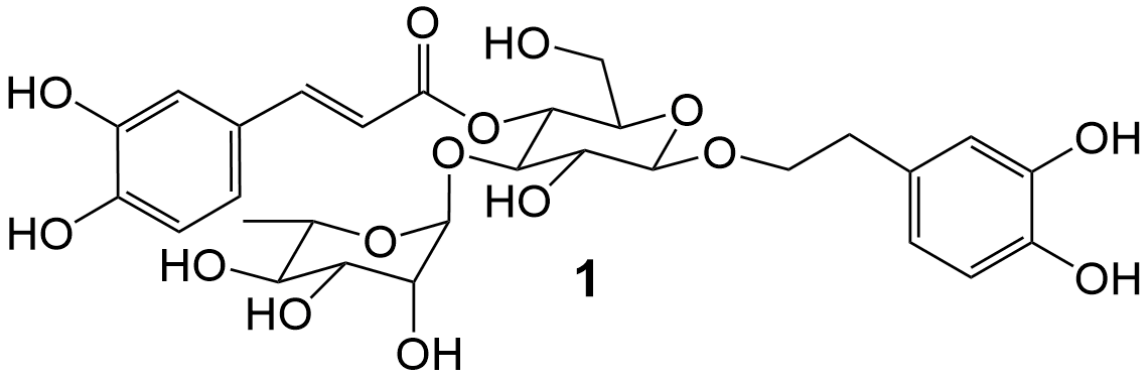


Figura 1. Estrutura química do verbascosideo

Agradecimentos/Acknowledgments

This research was supported by CAPES, CNPq and FAPESP(2024/00915-3).

Chemical profile and antimicrobial potential of the hexane phase from Melaleuca viminalis leaves

Ana Clara Lima Nunes Silva (PG)[1], Maria Teresa Saccuti Vidal (IC)[1], Marisi Gomes Soares (PQ)[2], Francisco Ozório Bessa Neto (PG)[1], Rodrigo Cayô da Silva (PQ)[1], Patricia Sartorelli (PQ)*[1].

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Palavras Chave:*Phloroglucinols,dereplication,GNPS,antimicrobial activity,Staphylococcus aureus*

Highlights

LC-MS/MS–GNPS dereplication revealed phloroglucinol-rich hexane fractions of*Melaleuca viminalis*with strong antimicrobial activity against*Staphylococcus aureus*, including MRSA.

Resumo/Abstract

Melaleuca viminalis(MV), a species belonging to the Myrtaceae family and formerly described as*Callistemon viminalis*, has undergone taxonomic reorganization, with all species of the genus*Callistemon*now classified as*Melaleuca*. This species exhibits a wide diversity of secondary metabolites, with phloroglucinols standing out due to their marked structural diversity and high biological potential. Previous studies have reported the antimicrobial activity of phloroglucinols isolated from MV, highlighting their relevance in the context of increasing bacterial resistance to conventional antibiotics. In this study, hexane partition fractions obtained from MV leaf extract (MVFH-1 to MVFH-11) were dereplicated by LC-MS/MS in combination with the GNPS platform., and their antimicrobial activity was evaluated by disk and well diffusion assays against ATCC, clinical, and resistant strains of*Acinetobacter baumannii*,*Enterococcus faecalis*,*Escherichia coli*,*Klebsiella pneumoniae*,*Pseudomonas aeruginosa*,*Staphylococcus aureus*(ATCC and MRSA), and*Enterobacter cloacae*. GNPS2 analysis enabled the annotation of six compounds, including three phloroglucinols: nor-semimyrtucommulone, rhodomyrtone A, and hyperjaponol A. In addition, two non-annotated clusters exhibited fragmentation patterns consistent with phloroglucinols, suggesting the presence of additional compounds from this class. The fractions showed more pronounced antimicrobial activity against*S. aureus*, including the resistant MRSA strain. Notably, fractions MVFH-1 to MVFH-7 concentrated the observed activity, displaying robust inhibition zones ranging from 11.4 to 24.1 mm, indicating the promising antimicrobial potential of compounds present in these fractions, particularly against resistant*S. aureus*strains.

Agradecimentos/Acknowledgments

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Chemical Profile of Essential Oils from Piper marginatum and Lippia origanoides Using GC-MS Combined with Multivariate Statistical Analysis

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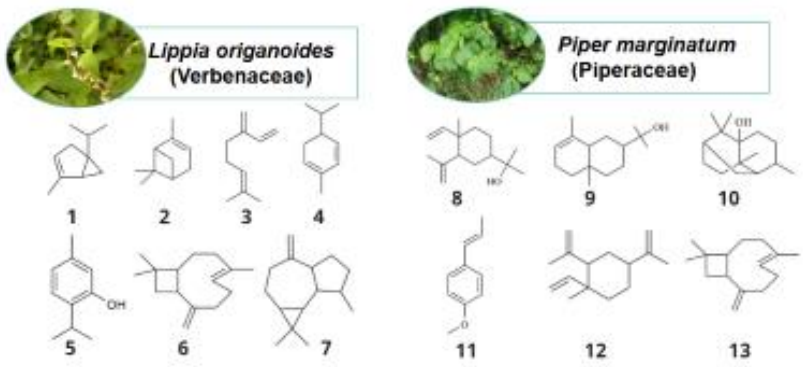
Palavras Chave:*Essential oils; Piper marginatum; Lippia origanoides; GC-MS; Multivariate Analysis*

Highlights

GC-MS and Multivariate Analysis differentiated essential oils from fresh and dried*Piper marginatum*and*Lippia origanoides*, revealing the predominance of mono and sesquiterpenes.

Resumo/Abstract

*Lippia origanoides*Kunth (Verbenaceae) is popularly known as “alecrim pimenta” and used in folk medicine for the treatment of skin conditions, as well for digestive and respiratory disorders. Essential oils of this species are rich in monoterpenoids such as carvacrol and thymol, with antimicrobial activity.[1–3]*Piper marginatum*Jacq. (Piperaceae) is a plant used in Brazilian folk medicine for its analgesic, anti-inflammatory, hemostatic, and wound-healing properties.[4–5] In this study, GC-MS coupled with multivariate analysis was employed to characterize and differentiate essential oils obtained from fresh and dried plants of both species. Essential oils were extracted by steam distillation and analyzed using GC-MS with an HP-5MS column. The oven program was set as follows: 0 °C for 2 min, then increased at 5 °C/min to 200 °C and held for 2 min, followed by a range of 50 °C/min to 250 °C and held for 1 min. Compounds were identified based on the NIST library, mass spectrometry data, and Kovats retention index, determined by injection of standard hydrocarbons under the same analytical conditions. Therefore, supervised multivariate statistical analysis by PLS-DA[6,7] was developed separately for each type of plant to investigate the composition variability according to the type of extraction. Analysis revealed that the essential oil of fresh*L. origanoides*was rich in α-thujene (1), α-pinene (2), β-myrcene (3), and α-phellandrene (4), whereas the essential oil from the dried plant has high amounts of thymol (5), caryophyllene (6), and aromandendrene (7). For*P. marginatum*, the essential oil of the fresh plant contained elemol (8), α-eudesmol (9), and patchoulol (10), while that of the dried plant had anethole (11), β-elemene (12), and caryophyllene (13) in high amounts. These compositional changes highlight the influence of plant processing on essential oil profiles, which may impact their biological activities and potential applications in pharmaceuticals and cosmetics.



Essential oil constituents of fresh and dried Lippia origanoides and Piper marginatum

Agradecimentos/Acknowledgments

This study was financially supported by the Livealoe company, FINEP (Reference: 0558/21) and FUNCAP (Reference: 01986340/2021), Brazil.

Chemical profiling of cannabinoids from different Cannabis sativa L. varieties by Liquid Chromatography coupled to Mass Spectrometry (LC–MS)

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Palavras Chave:*Cannabis sativa L.,phytocannabinoids,LC–QTOF–MS/MS,exploratory analysis,qualitative profiling*

Highlights

LC–QTOF–MS/MS qualitatively profiled Feno Swiss and Northern Lights resins, revealing shared and specific cannabinoids; isomeric compounds require complementary techniques for precise identification.

Resumo/Abstract

*Cannabis sativa*L. is a chemically complex plant with its therapeutic potential mainly attributed to its phytocannabinoids. The concentration and profile of these compounds may vary due to genetic and environmental factors, emphasizing the need for reliable analytical methods for their identification and quantification. In this context, cannabinoids were qualitatively characterized using liquid chromatography coupled to quadrupole time-of-flight tandem mass spectrometry (LC–QTOF–MS/MS) as an exploratory analysis, providing preliminary information to support the future development of a quantitative method applicable to cannabis-derived samples produced by patient associations. In this study, decarboxylated Northern Lights and non-decarboxylated Feno Swiss resins were analyzed by LC–QTOF–MS/MS, using positive ionization mode and base peak chromatograms (BPC) for cannabinoid detection. Qualitative analysis identified both common and variety-specific cannabinoids. Signals compatible with CBN were observed in both varieties. Other signals could correspond to isomeric cannabinoids, including CBCA, CBDA, THCA, CBD, Δ8-THC, Δ9-THC, CBC, CBL, or CBCT, but m/z alone cannot unambiguously distinguish among them. CBT was detected exclusively in Feno Swiss, whereas 11-nor-9-carboxy-THC and CBNA were identified only in Northern Lights, indicating variety-dependent cannabinoid profiles likely influenced by genetic background and decarboxylation status. These differences are particularly relevant, as variations in cannabinoid composition may directly affect the therapeutic potential, safety, and reproducibility of cannabis-derived products used by patients. However, accurately linking these compositional differences to specific compounds was limited, as several cannabinoids exhibit identical m/z values, highlighting the need for complementary techniques to achieve accurate structural elucidation.

Agradecimentos/Acknowledgments

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Chemical prospection of polysaccharides and lipids from the Amazonian wild mushroom Tylopilus sp.

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Palavras Chave:*Amazon,macrofungi,Tylopilus,polysaccharides,fatty acids.*

Highlights

Chemical prospection revealed polysaccharides and fatty acids in Amazonian*Tylopilus*sp. A β-(1→3),(1→6)-glucan was identified by ^{13}C NMR, highlighting biotechnological potential.

Resumo/Abstract

The genus*Tylopilus*(Boletaceae) comprises basidiomycete mushrooms with wide geographical distribution in tropical and temperate regions. Species of this genus are predominantly ectomycorrhizal and play an important ecological role in forest ecosystems, but remain poorly studied in neotropical environments. In the Amazon Rainforest,*Tylopilus*occurs mainly in sandy soils, contributing to nutrient cycling and fungal biodiversity. From a chemical perspective,*Tylopilus*mushrooms are of interest due to the presence of polysaccharides, lipids, and other metabolites with nutritional and biotechnological potential. Considering the scarcity of chemical studies on polysaccharides from this genus, this work aimed to perform the chemical prospection of these biomolecules from a species collected in the Amazon biome. Polysaccharides were obtained by aqueous extractions at different temperatures (~ 10 and 96 °C), yielding the extracts*Tyl*-AF and*Tyl*-AQ, followed by ethanolic precipitation (1:1, v/v). The precipitates (*Tyl*-1PEAF and*Tyl*-1PEAQ) were separated by centrifugation and lyophilized. Chemical characterization was carried out using chromatographic and spectroscopic techniques (GC-MS, NMR, and HPSEC-RID-LS). ^{13}C NMR analysis of the*Tyl*-1PEAQ fraction indicated a β-glucan (*Tyl*-BG1) composed of glucose units linked by β-(1→3) and β-(1→6), similar to biologically active polysaccharides. In addition, basidiomes of*Tylopilus*sp. were analyzed for fatty acid composition by GC-MS after derivatization to methyl esters (FAMEs). Overall, the results demonstrate the chemical potential of Amazonian*Tylopilus*sp. as a source of structurally relevant polysaccharides and contribute to the knowledge and valorization of neotropical fungal biodiversity, indicating promising nutritional and biotechnological applications.

Agradecimentos/Acknowledgments

This study was supported by the Goiás State Research Support Foundation (Fundação de Amparo à Pesquisa do Estado de Goiás- FAPEG) (Grant numbers: 202310267000034 and 202310267001406).

Chirality in insect communication: its role in behavioural responses and challenges for pheromone identification.

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Palavras Chave:*Semiochemicals,Pheromones Insects Chirality Chromatography*

Highlights

Chirality plays a fundamental role in nature, as differences in absolute configuration can alter both the odour of a molecule and its biological activity.

Resumo/Abstract

Chirality plays a fundamental role in nature, as differences in absolute configuration can alter both the odour of a molecule and its biological activity, including its effects on insect behaviour. In insects, olfactory perception is essential for locating mates, finding food and shelter, and detecting potential threats, guaranteeing species survival. Odor perception is typically a complex process that involves blends of multiple compounds rather than single molecules. The scent of mango inflorescences, for example, is readily recognized by humans after initial exposure and is mainly associated with monoterpenes such as myrcene and 3-carene, as well as esters like methyl and ethyl benzoate. Similarly, the weevil*Sternochetus mangiferae*can recognize the odour of its preferred host plant, the mango tree. This insect is attracted to a synthetic blend of eight mango volatiles, which includes (*S*)-linalool. However, when the same blend is prepared using (*R*)-linalool or a racemic mixture, it loses its attractiveness, highlighting the importance of chirality in insect olfactory responses. Chirality is also critical in pheromone-mediated communication. The stink bug*Nezara viridula*produces two sesquiterpenes, (4S)-cis- and (4S)-trans-(Z)-bisabolene epoxide, as components of its sex pheromone, and females respond specifically to the natural stereochemical configuration produced by males.*Euschistus heros*males produce the sex pheromone methyl (2*R*,6*R*,10*S*)-trimethyltridecanoate. Females show strong responses to the naturally occurring stereoisomer and to racemic mixtures. In this presentation, we will discuss the importance of chirality in insect chemical communication, as well as the challenges associated with determining the absolute configuration of pheromone molecules. These compounds are typically produced in extremely small quantities, often at the nanogram level, and occur within complex chemical mixtures, making their identification particularly challenging.

Agradecimentos/Acknowledgments

CNPq, FAP-DF, INCT BioInova, Embrapa

Cocultivo de bactérias associadas a corais como estratégia para indução de metabólitos bioativos

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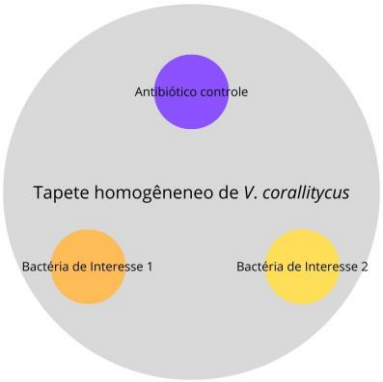
Palavras Chave:*Bactérias Marinhas,Cocultivo Microbiano,Corais,Metabólitos Secundários,Metabolômica*

Highlights

Antagonistic interactions guide bioactive metabolite discovery. Coral-associated bacteria integrate microbiology and chemical ecology.

Resumo/Abstract

Os organismos marinhos constituem ecossistemas altamente complexos, nos quais comunidades microbianas associadas estabelecem redes dinâmicas de interações ecológicas e moleculares essenciais à manutenção da saúde do hospedeiro. Nesse cenário, cepas do gênero*Vibrio*, frequentemente associadas a estados de disbiose e patogenicidade em organismos marinhos, destacam-se pela expressão de genes de virulência envolvidos em processos como adesão, motilidade, secreção de toxinas e aquisição de nutrientes. O cocultivo de cepas bacterianas isoladas com*Vibrio*constitui, portanto, uma estratégia experimental relevante para investigar interações antagonistas capazes de interferir na expressão e/ou na funcionalidade dos fatores de virulência vibrionais. A competição por recursos e a exposição a metabólitos produzidos pelas bactérias isoladas podem exercer pressão seletiva sobre*Vibrio*, resultando na inibição do crescimento ou na repressão de vias regulatórias associadas à patogenicidade. Dessa forma, neste projeto foi realizado um screening de bactérias isoladas de corais na busca-se de potenciais antagonistas de Vibrio.Os ensaios de cocultivo foram realizados a partir do plaqueamento homogêneo da cepa*Vibrio*BAA-450, formando um tapete bacteriano. Sobre essa superfície, foram depositadas alíquotas de 10 µL de cultivo líquido de diferentes bactérias isoladas de corais, permitindo a avaliação de interações antagônicas por meio da formação de zonas de inibição. Uma gota contendo solução de antibiótico foi usado na placa como controle positivo. As cepas que apresentaram halo de inibição de crescimento da*Vibrio*foram submetidas à processo de extração de metabólitos com posterior análise por cromatografia líquida acoplada à espectrometria de massas. Dessa forma, o projeto contribuirá para o avanço do conhecimento microbiológico e químico sobre bactérias associadas a corais, além de fornecer bases para a identificação de novos metabólitos bioativos de interesse biotecnológico.



Esquema de deposição do cocultivo entre a V. Corallitycus e as bactérias de interesse

Agradecimentos/Acknowledgments

Os autores agradecem à FAPESP pela bolsa (processo 2025/19861-3) e projeto Jovem Pesquisador (2024/05211-4).

Co-culture-Driven Enhancement of 10,11-Dehydrocurvularin Production by Endophytic Fungi from Opuntia ficus-indica

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Palavras Chave:*Curvularia pseudointermedia,curvularin-type metabolite,bioactive metabolite,co-culture strategies,Brazilian Northeast host plants*

Highlights

Co-culture strategies as an effective approach to stimulate the biosynthesis of bioactive specialized metabolites by endophytic fungi

Resumo/Abstract

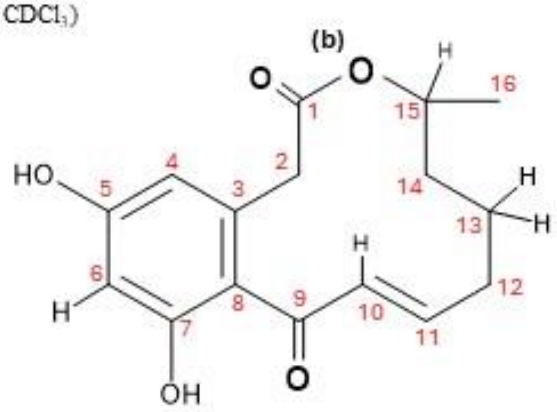
Opuntia ficus-indica, native to Mexico, is popularly known in Bahia-BR as “palma-forrageira”. This cactus is essential for the Brazilian Semi-arid region due to its adaptation to dry climates and is used in folk medicine for the treatment of inflammation and diabetes[1]. Endophytic fungi inhabit the internal tissues of plants and can enhance host survival through the production of specialized metabolites[2]. Microbial co-culture is a powerful strategy for inducing the biosynthesis of otherwise silent bioactive metabolites. As part of our ongoing bioprospecting efforts targeting endophytic fungi isolated from host plants to the Brazilian Northeast, we report herein the isolation, molecular identification, and chemical characterization of two endophytic fungal strains from*O. ficus-indica*:*Curvularia pseudointermedia***P10**and*Schizophyllum radiatum*P1.They were isolated according to previously established protocols and identified by amplification of the translation elongation factor 1-α (TEF1-α) region using EF1-1018/EF1-1620 primers. The fungi were cultivated in both single and co-cultures, established through fungus-fungus and fungus-bacterium confrontation with*Staphylococcus aureus*. Ethyl acetate extracts were analyzed by UHPLC-DAD to detect metabolites produced or significantly upregulated in co-cultures. Guided by chromatographic analysis, the polyketide 10,11-dehydrocurvularin (**1**) was isolated and chemically characterized using 1D and 2D NMR spectroscopy. This curvularin-type metabolite was produced in both cultures involving**P10**. However, its biosynthesis was enhanced under confrontation conditions. Compound**1**is known for its antitumor and anti-inflammatory activities[3]. Overall, our results highlight co-culture strategies as an effective approach to stimulate the biosynthesis of bioactive specialized metabolites by endophytic fungi.

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(a) Table 1. Compound **1** ^{13}C NMR (125MHz, $CDCl_3$) and ^{1}H NMR (500MHz, $CDCl_3$)

Position	δC [ppm]	δH [ppm] (mult, J[Hz])
1	173.3	-
2	44.2	a: 4.05 (d, 20); b: 3,53(d, 20)
3	137.7	-
4	114.0	6.25 (d, 5)
5	161.4	-
6	103.5	6.22 (d, 5)
7	166.5	-
8	114.3	-
9	196.3	-
10	131.6	6.58-6.69 (m)
11	148.3	
12	32.8	2.30-2.37 (m)
13	24.2	1.68-.162 (m)
14	33.9	1.01-1.88 (m)
15	73.2	4.89-4.86 (m)
16	19.9	1.25 (d, 5)

(b)



(a) 10,11-dehydrocurvularin NMR data; (b) Structure of 10,11-dehydrocurvularin

Cytotoxic activity of Bacopa scoparioides leaves essential oil

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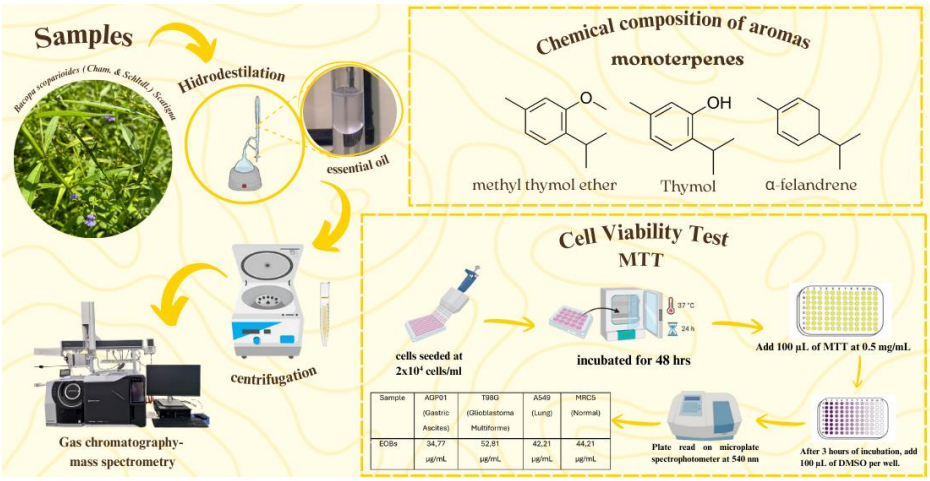
Palavras Chave:*Plabntaginaceae; monoterpines; Biodiversity; MTT.*

Highlights

Thymol-rich essential oil from*Bacopa scoparioides*shows moderate invitro cytotoxic activity in human cell lines.

Resumo/Abstract

Bacopa scoparioides(Cham. & Schltdl.) Scatigna is knows as pataqueira, this specie is an aromatic widely used by traditional communities in the Northern region of Brazil, and has attracted scientific interest due to its biological potential, especially related to volatile secondary metabolites. The present work aims to characterize the chemical composition of*B. scoparioides*leaves essential oil (BsEO) and evaluate its in vitro cytotoxic activity. The leaves were collected in the municipality of Acará, Pará. A voucher was incorporated into the Herbarium of the State University of Pará (MFS-11520). The dried leaves were subjected to hydrodistillation in a Clevenger apparatus. Chemical characterization was performed by gas chromatography coupled to mass spectrometry (GC-MS). Cytotoxic activity was evaluated by the MTT colorimetric assay against human cell lines A549 (lung adenocarcinoma), AGP01 (gastric ascites), T98G (glioblastoma), and MRC5 (human lung fibroblast). The essential oil yield was 5.8%. Forty constituents were identified, thymol (46.95%), methylthymol ether (33.38%), and α-phellandrene (9.52%) werer the main constituents, configuring a chemical profile rich in phenolic monoterpenic compounds. The BsEOdisplayed moderate cytotoxicity in all cell lines: T98G (IC50 52.81 µg/mL), AGP-01 (IC50 34.77 µg/mL), A549 (IC50 42.21 µg/mL), and MRC5 (IC50 44.21 µg/mL). The observed cytotoxicity may be associated with the high concentration of thymol and the possible synergistic action between the major constituents of the oil. The BsEO oil has a well-defined chemical composition and moderate cytotoxic activity, contributing to the chemical and biological knowledge of the specie and indicating its potential as a source of bioactive compounds, although further studies are needed for a better understanding of the mechanisms of action and biological selectivity.



Cytotoxic activity of Bacopa scoparioides leaves essential oil

Agradecimentos/Acknowledgments

We thank CNPq for funding this research through Pró-Amazônia (Call for Proposals 19-2024). We also thank PADAP research group, LAQUIPRON, CMABio, and UEPA for their institutional support.

Cytotoxicity of leaf and resin essential oils from Protium heptaphyllum (breu-branco) in the Amazon Region

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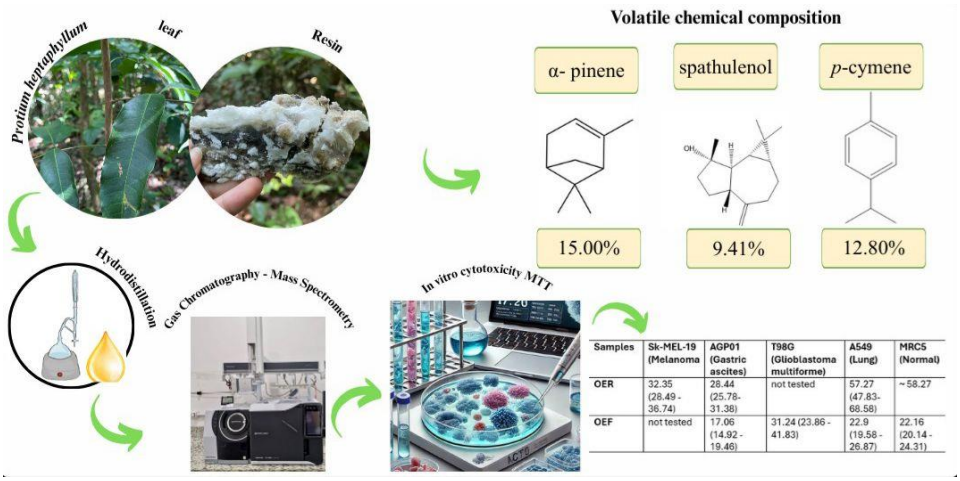
Palavras Chave:*Protium heptaphyllum,Essential oils,Cytotoxicity,MTT assay*

Highlights

The essential oils of*P. heptaphyllum*displayed low cytotoxicity against tumor cell lines. EO OL OR

Resumo/Abstract

Protium heptaphyllum(Burceraceae), popularly known as breu-branco, is an aromatic medicinal plant that produces essential oil (EO) present in its leaves, bark and resins. The aim of this study was to evaluate the cytotoxic activity of the essential oil of its resins (EOR) and leaves (EOL). The resin sample were obtained in the commercial market of Jurunas (Belém-PA). The leaves were collected in the municipality of Acará-PA. A leaf sample incorporated into the herbarium Marlene Freitas da Silva (MFS-11519). The samples were dried and hydrodistilled modified Clevenger extractor. The chemical composition was analyzed by GC-MS. The cytotoxicity of the EO was evaluated by the MTT assay against the tumor cell lines Sk-MEL-19 (melanoma), AGP01 (gastric ascites), A549 (lung carcinoma), T98G (glioblastoma multiforme) and MRC5 (human lung fibroblast). EO yields were 2.09% (EOR) and 0.34% (EOL). The main constituents (> 5%) were α-pinene (EOR: 15.0%; EOL: 0%), β-pinene (EOR: 6.2%; EOL: 0%),*p*-cimene (EOR: 12.8%; EOL: 0%), limonene (EOR: 12.2%; EOL: 0%), α-terpineol (EOR: 5.6%; EOL: 0%), spathulenol (EOR: 0%; EOL: 9.41%), (*E*)-caryophyllene (EOR: 0%; EOL: 8.26%), α-copaene (EOR: 0%; EOL: 7.41%), viridiflorol (EOR: 0%; EOL: 7.31%), α-cadinol (EOR: 0%; EOL: 6.63%), epi-α-murrolol (EOR: 0%; EOL: 5.98%). EOR and EOL for the cell lines tested: Sk-MEL-19 (EOR: CI_{50} 32.35 µg/mL; EOL: untested), AGP01 (EOR: CI_{50} 28.44 µg/mL; EOL: CI_{50} 17.06 µg/mL), A549 (EOR: CI_{50} 57.27 µg/mL; EOL: CI_{50} 22.9 µg/mL), T98G (EOR: untested; EOL: T98G: CI_{50} 31.24 µg/mL) and MRC5 (EOR: CI_{50} 58.27 µg/mL; EOL: CI_{50} 22.16 µg/mL) based literature that only EO with IC50 < 30 µg/mL against tumor strains are promising anti-cancer and a value (≥2) as a favorable selectivity index. That EOR and EOL showed CI<30 µg/mL against AGP01 (EOR: 28.44 µg/mL, SI=2.04; EOL: 17.06 µg/mL) and A549 (EOL: 22.9 µg/mL). These results indicating of EOR and EOL selective anticancer potential.



Cytotoxicity of leaf and resin essential oils from Protium heptaphyllum (breu-branco) in the Amazon

Agradecimentos/Acknowledgments

Acknowledgments: To the National Council for Scientific and Technological Development (CNPq) for funding this research through the Pró-Amazônia program (Call for Proposals 19-2024).

DAFdiscovery: uma plataforma integrada para correlação entre espectrometria de massas, RMN e bioatividade em metabolômica e produtos naturais

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Palavras Chave:*DAFdiscovery; Data Fusion*

Highlights

Integração de dados de**LC-MS/MS, RMN e bioatividade**

Implementação do**STOCSY**para correlação direta entre sinais

Visualizações interativaspara inspeção crítica e validação ponto a ponto dos resultados

Resumo/Abstract

A integração de dados provenientes de espectrometria de massas, ressonância magnética nuclear (RMN) e ensaios de bioatividade é um desafio em metabolômica e química de produtos naturais, especialmente em estudos envolvendo amostras complexos e múltiplos lotes experimentais. Nesse contexto, apresentamos o**DAF*discovery***, uma plataforma computacional interativa desenvolvida em Python e Streamlit, projetada para integrar, correlacionar e visualizar dados analíticos e biológicos de forma facilitada.

O**DAF*discovery***permite a submissão de diferentes tipos de dados experimentais, incluindo tabelas de features de LC-MS/MS, dados de RMN (espectros em*high-resolution*) e resultados quantitativos de bioatividade, associados a um arquivo de metadados padronizado. A plataforma identifica automaticamente o tipo de dado carregado, executa rotinas específicas de pré-processamento e garante a correspondência consistente entre amostras, minimizando erros de integração.

O sistema implementa o método**STOCSY**para correlacionar sinais espectrais com variáveis biológicas ou químicas de interesse. O usuário pode realizar análises automáticas utilizando a bioatividade como variável diretora ou executar análises manuais, selecionando qualquer feature como driver. Os resultados são apresentados por meio de visualizações interativas, incluindo gráficos de correlação, scatter plots e representações espectrais, permitindo inspeção ponto a ponto e validação crítica dos dados. Disponível aqui: https://dafdiscovery.streamlit.app/

A plataforma oferece ainda exportação dos resultados, facilitando a rastreabilidade, a documentação e a comunicação científica. O**DAF*discovery***tem sido aplicado em estudos de desreplicação, priorização de metabólitos bioativos, integração inter-lote e exploração do espaço químico de extratos naturais, destacando-se como uma ferramenta flexível para pesquisas em metabolômica, produtos naturais e biotecnologia, com ênfase em interpretação assistida, e não em automação cega.

Agradecimentos/Acknowledgments

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Desenvolvimento de Creme Cosmético para Prevenção da Descamação e Proteção do Couro Cabeludo Durante o Alisamento Químico

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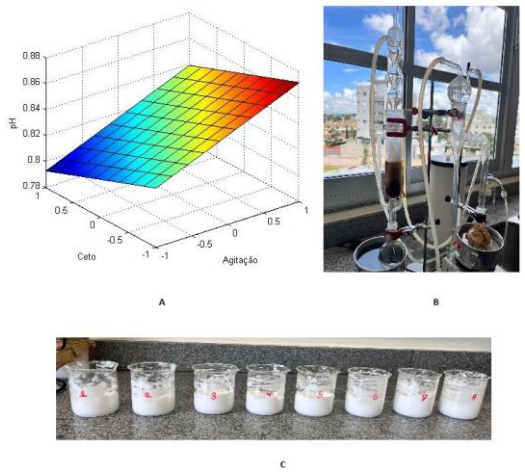
Palavras Chave:*Calendula officinalis,Formulação cosmética,Proteção do couro cabeludo,Alisamento químico,pH*

Highlights

A protective hair cream for scalp during chemical straightening was developed, using*C. officinalis*as anti-inflammatory. pH and density was studied.

Resumo/Abstract

Este trabalho descreve o desenvolvimento de um creme cosmético para proteger o couro cabeludo durante procedimentos de alisamento químico, que frequentemente causam irritação e descamação devido a agentes agressivos e altas temperaturas. O estudo focou na criação de uma formulação à base de creme capilar, utilizando*Calendula officinalis*como ativo principal por suas propriedades calmantes e anti-inflamatórias. Vaselina foi adicionada como agente oclusivo para criar uma barreira protetora, e álcool cetoestearílico (ceto) como agente estruturante da emulsão, com o teor de água ajustado conforme sua concentração. Oito formulações experimentais foram preparadas utilizando um planejamento fatorial 2^3, variando unicamente a concentração de vaselina (0% e 1,5%), ceto (4% e 6%) e o modo de agitação (normal e turbo). A caracterização físico-química incluiu a determinação do pH e da densidade. Os valores de pH, que variaram entre 2,48 e 2,54, indicaram baixa variabilidade e boa reprodutibilidade, sendo compatíveis com produtos que neutralizam a alcalinidade dos alisantes. Observou-se que a adição de vaselina e o aumento da concentração de ceto tendem a aumentar o pH, enquanto o aumento da agitação o diminui. Interações negativas significativas entre agitação e as concentrações de vaselina e ceto foram notadas, resultando em uma diminuição do pH maior do que o esperado pela agitação isoladamente. A agitação parece ser o fator com maior influência cruzada no pH, mas é necessário averiguar o efeito do ácido lático adicionado. Geralmente, o meio torna-se mais alcalino com maior agitação e menor teor de ceto. Quanto à densidade, ela diminui com o aumento da agitação e do ceto, mas aumenta significativamente com a vaselina. As interações entre agitação e ceto/vaselina na densidade também foram negativas. Os resultados sugerem que o creme desenvolvido tem potencial como produto auxiliar na proteção do couro cabeludo durante o alisamento químico.



(A) Superfície de resposta; (B) Extração de C. officinalis com Sohxlet e Clevenger; (C) Formulações.

Agradecimentos/Acknowledgments

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Development and characterization of antimicrobial films containing nanoemulsion of Piper aduncum L. essential oil.

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Palavras Chave:*Biopolymer,Natural food preservative,Active packaging*

Highlights

Active biopolymer films containing a nanoemulsion of P. aduncum essential oil have been shown effective against fungi, capable of extending the shelf life of bread by up to 12 days.

Resumo/Abstract

Constant efforts have been made to develop more sustainable food packaging that can optimize the preservation of perishable foods, especially bakery products. This study aimed to develop, characterize, and evaluate the antimicrobial efficacy of biopolymeric films incorporating a nanoemulsion of*P. aduncum*essential oil for bread preservation. The mechanical properties of the biofilms, such as tension, deformation, and toughness, were evaluated as a function of the amount of plasticizer used. Images of the film surface and fracture edge were also obtained. Resistance to colonization by filamentous fungi (*Penicillium adametzii, Aspergillus flavus,*and*A. niger*), as well as the influence of the active film on the shelf life of bread slices, were also evaluated. The essential oil of*P. aduncum*, used in this study, had a yield of 1.75%, and the main constituents identified were dillapiole (80.26%),*E*-caryophyllene (5.45%), D-germacrene (1.67%), and myristicin (1.83%). The polymeric films obtained with the incorporation of the oil were translucent, odorless, and of varying thickness. Furthermore, it was observed that the use of glycerol up to 0.8% (w/w, carboxymethylcellulose base) improved the material's resistance and conferred greater elasticity. Tests also revealed that the polymeric film containing 0.8% glycerol showed resistance to microbial colonization, increasing the food shelf life by 12 days. These results may provide alternatives to conventional methods of microbial control in bakery products, reducing economic losses in the food sector and intoxications from the ingestion of contaminated food or excess preservatives.

Agradecimentos/Acknowledgments

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Diterpenes and triterpenes with anthelmintic activity from leaves of Guarea macrophylla Vahl (Meliaceae)

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Palavras Chave:*Guarea macrophylla, diterpenes, triterpenes, anthelmintic activity,Guarea macrophylla,Diterpenes,Triterpenes,Anthelmintic activity*

Highlights

The*G. macrophylla*hexane leaf extract showed anthelmintic activity*in vitro*. Silica chromatography of bioactive fractions yielded fatty acids, four diterpenes, and two triterpenes.

Resumo/Abstract

The Meliaceae family, belonging to the order Sapindales, comprises approximately 51 genera and 1,400 species. In recent years, Meliaceae species have attracted increasing scientific interest due to their remarkable ability to produce bioactive secondary metabolites, particularly terpenoids. These compounds exhibit a broad spectrum of biological activities, including insecticidal, fungicidal, bactericidal, and antiviral effects. Notably, several studies have recently reported the anthelmintic potential of terpenoids, especially di- and triterpenes. In this context, the hexane extract obtained from the leaves of*Guarea macrophylla*showed*in vitro*activity against*Schistosoma mansoni*at a concentration of 200 mg/mL. To identify the bioactive constituents, the extract was subjected to silica gel column chromatography using mixtures of hexane:EtOAc as eluents, yielding ten groups (A–J). After*in vitro*anthelmintic evaluation, groups B–I exhibited significant activity and were subsequently analyzed by MS and NMR techniques. As a result, in addition to several fatty acids, four diterpenes—phytol (**1**), kaurenoic acid (**2**), isopimara-7,15-dien-3β-ol (**3**), and isopimara-7,15-dien-3-one (**4**)—and two triterpenes—3β-hydroxy-cycloart-24-en-23-one (**5**) and (23S)-hydroxy-cycloart-24-en-3-one (**6**)—were identified in the bioactive groups. Except for phytol (**1**), previously reported as active against*S. mansoni*, this study represents the first report of anthelmintic activity for compounds**2–6**from*G. macrophylla*.

Agradecimentos/Acknowledgments

I would like to acknowledge the support from**CAPES, FAPESP, UFABC, and PPGCTQ**.

Effect of Immersion of Brazil Nuts in an Essential Oil Blend on Aspergillus flavus Growth and Aflatoxin B1 Production

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Palavras Chave:*Aspergillus flavus,Cymbopogon citratus,Eugenia caryophyllata,Aflatoxin B1,Brazil nuts*

Highlights

Application of essential oil blend reduced*A. flavus*growth on Brazil nuts Lower concentrations increased aflatoxin B1 production Higher concentrations reduced fungal growth and toxin levels

Resumo/Abstract

Brazil nuts, the edible seeds of*Bertholletia excelsa*H.B.K., are highly susceptible to contamination by*Aspergillus flavus*, a major producer of aflatoxin B1 (AFB1) during post-harvest handling and storage, representing a significant food safety concern. This study evaluated the effect of applying a 1:1 (v/v) blend of commercially available*Cymbopogon citratus*and*Eugenia caryophyllata*essential oils by immersion on fungal growth and AFB1 production by*A. flavus*isolated from Brazil nuts. The oil blend was added to an aqueous solution containing 0.3 mL/L Extravon®, and Brazil nuts (30 g, approximately five units) with intact shell were immersed in this solution at concentrations corresponding to 10, 50, and 100 times the minimum inhibitory concentration (MIC), followed by inoculation with 5 × 10^5 conidia/mL. Samples were incubated at 25 °C for 19 days in triplicate. Thiabendazole was used as a positive control, and nuts inoculated only with conidia as negative control. Fungal growth was evaluated qualitatively, and AFB1 production was quantified by HPLC with fluorescence detection. The MIC of the essential oil blend was 800 µg/mL, while the MIC of thiabendazole was 0.125 µg/mL. Qualitative analysis showed a marked reduction in fungal growth at 50× and 100× MIC. However, quantitative analysis revealed higher AFB1 levels at 10× MIC (10.48 ± 3.97 ng/g), with lower levels observed at higher concentrations (4.61 ± 0.82 ng/g at 50× and 3.38 ± 1.42 ng/g at 100× MIC). These findings suggest that the essential oil blend can induce metabolic stress in*A. flavus*at lower tested concentrations, leading to increased aflatoxin production, whereas higher concentrations effectively reduce both fungal growth and AFB1 levels, emphasizing the importance of concentration optimization for post-harvest fungal control strategies in Brazil nuts.

In vitro evaluation of the antioxidant and antiglycation activity of the ethanolic extract of jambolan (Syzygium cumini) seeds

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Palavras Chave:*Bioactives,Glycation,Syzygium cumini*

Highlights

Ethanol extract of*Syzygium cumini*seeds, an agroindustrial residue, exhibited*in vitro*antioxidant and antiglycation activity, with phytotherapeutic potential and alignment with SDGs 3 and 12.

Resumo/Abstract

The seeds of jambolan (*Syzygium cumini*), a fruit native to Asia and widely cultivated in Brazilian territory, are agroindustrial residues rich in phenolic compounds, such as flavonoids and tannins[1], and can be used as secondary metabolites in the treatment of diseases associated with oxidative and carbonyl stress, due to their ability to capture reactive species and inhibit the formation of Advanced Glycation End-products (AGEs)[2]. The objective of this study was to evaluate the antioxidant and antiglycation activity of the ethanolic extract of jambolan seeds (EEJS). The EEJS was obtained using a Soxhlet extractor, with a yield of 8.23%. The Total Phenolic Contents (TPC) was determined by the Folin-Ciocalteu method, the antioxidant activity by the 2,2-diphenyl-1-picrylhydrazyl (DPPH•) and Ferric Reducing Antioxidant Power (FRAP) assays, and the antiglycation activity by the*in vitro*Bovine Serum Albumin (BSA) with glucose and fructose (GF) system. As a result, EEJS showed a TPC value of 5785.6 ± 28.3 mg Gallic Acid Equivalents/g of dry extract. An IC_{50} of 5.53 ± 0.03 µg/mL was obtained for the DPPH• assay, and in the FRAP assay, a value of 1128.67 ± 2.75 mg Trolox Equivalent/g was obtained at a concentration of 5 µg/mL. For the BSA/GF systems, the extract proved effective in inhibiting the formation of AGEs. The results obtained reinforce the promising potential of the*S. cumini*seed extract as a possible source of phytotherapeutics, with significant antioxidant and antiglycation activities in*in vitro*systems. Furthermore, this work contributes to SDGs 3 and 12 by promoting responsible consumption practices through the reuse of agro-industrial residues, good health and well-being.

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Agradecimentos/Acknowledgments

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In vitro growth inhibition of the leaf-cutting ants' symbiotic fungus Leucoagaricus gongylophorus by different crude extracts.

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Palavras Chave:*Leucoagaricus,Pycnoporus,Atta,Lavandula,ants*

Highlights

Among all tested samples, fractions of the extract of lavender (*Lavandula dentata*) and the fungus*Pycnoporus sp*. exhibited the highest inhibitory effects on the growth of*Leucoagaricus gongylophorus*.

Resumo/Abstract

Leaf-cutting ants of the genera*Atta*and*Acromyrmex*are major agricultural pests in Brazil, causing significant yield and economic losses. Their impact is driven by the cultivation of the symbiotic fungus*Leucoagaricus gongylophorus*, which is essential for colony survival. Current control strategies rely on non-biodegradable synthetic insecticides, leading to environmental contamination and mortality of non-target organisms. Thus, alternative approaches targeting the control of*L. gongylophorus*are of increasing interest. In this study, natural extracts were evaluated for their ability to inhibit the in vitro growth of*L. gongylophorus*. The assays were performed in Petri dishes containing 10 mL of culture medium, with extract concentrations ranging from 1.06 to 1.60 mg/mL. A 9mm agar plug previously colonized by the symbiotic fungus was placed at the center of each plate. The plates were incubated at 21 °C for 30 days, and DMSO, used to solubilize the extracts, was employed as the solvent control. Fungal growth inhibition was evaluated by measuring mycelial growth along five axes using*ImageJ*software. All experiments were conducted in quintuplicate. Growth inhibition rates were observed for: (**1**) fractions of the aqueous extract from the fruiting body of*Pycnoporus sp*. obtained by SPE-C_{18} - water (**100%**) and methanol (26%); (**2**) the acetone:methanol 1:1 v/v extract of the*Pycnoporus sp*. fruiting body (37%); (**3**) the ethyl acetate fraction obtained by liquid–liquid partitioning of decoction water from lavender essential oil extraction (**86%**); and (**4**) ethyl acetate fractions obtained by liquid–liquid partitioning of the*Pinus sp*. stem resin - extract water:ethanol 3:1 v/v (54%) and acid-base extraction (56%). These results demonstrate the strong inhibitory potential of fractions derived from*Pycnoporus sp*. and lavender (*Lavandula dentata*) against the growth of the leaf-cutting ants' symbiotic fungus*Leucoagaricus gongylophorus*.



Fruiting body of fungus Pycnoporus sp. collected at Embrapa Southeast Livestock.

Agradecimentos/Acknowledgments

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In Vitro leishmanicidal potential of clove: a comparative analysis of commercial samples of Syzygium aromaticum

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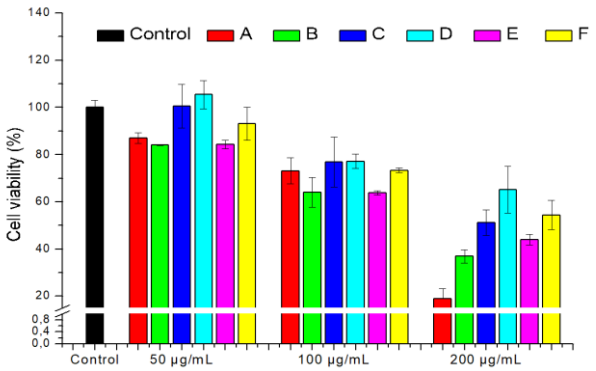
Palavras Chave:*Syzygium aromaticum,clove,L. amazonensis,eugenol,eugenyl acetate*

Highlights

Clove samples with high eugenol acetate content reduced the viability of*L. amazonensis*cells, demonstrating that raw standardization is crucial for the pharmaceutical viability of these extracts

Resumo/Abstract

Clove (*Syzygium aromaticum*) is an aromatic tree of the Myrtaceae family, rich in eugenol (phenylpropanoid), with significant industrial and pharmaceutical interest due to its biological properties. This study aimed to qualitatively evaluate clove samples from different commercial sources (**A-F**) to quantify the terpene eugenol and correlate this constituent with a possible antiparasitic action against promastigote forms of Leishmania protozoa. Samples were extracted in ethyl acetate via dynamic maceration. Analyses were performed by Gas Chromatography coupled with Mass Spectrometry (GC-MS), using SCAN mode for chemical composition determination and SIM mode for eugenol quantification. Samples were analyzed in triplicate, and results were evaluated based on the relative percentage of compounds and eugenol content. Subsequently,*S. aromaticum*extracts were dried and subjected to*in vitro*viability assays against*Leishmania amazonensis*, using the MTT method. The major compounds identified were eugenol, trans-caryophyllene, α-humulene, eugenyl acetate, and caryophyllene oxide. All samples were inactive at the lowest concentrations tested (>25 µg/mL); however, they showed selectivity at higher concentrations (50-200 µg/mL). Notably, samples**A**and**B**showed 81% and 63% reductions in parasite cell viability at 200 µg/mL, respectively. The results indicate that the superior leishmanicidal activity of sample**A**correlates with its elevated eugenyl acetate content (27.17%) relative to the other samples. While eugenol remains the primary constituent across all extracts, the variation in eugenyl acetate concentration suggests this compound plays a pivotal role in the toxicity observed against*L. amazonensis*promastigotes. In conclusion, the results highlight that raw material standardization and quality control are decisive factors in ensuring the safety, efficacy, and pharmaceutical viability of*S. aromaticum*extracts, especially in developing therapies for neglected diseases.



Cell viability graph obtained from the screening of extracts A–F against L. amazonensis promastigote

Agradecimentos/Acknowledgments

To the University Center of Paulínia (UNIFACP) for providing the laboratory.

Endophytic Talaromyces sp. P6 as a Source of Meroterpenoid with Anti-Leishmanial Potential

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Palavras Chave:*Endophytic fungi,Talaromyces,Antileishmanial activity,LC–HRMS,Specialized metabolites.*

Highlights

Metabolomics-guided isolation of the meroterpenoid austin reveals that the endophytic*Talaromyces*sp. P6 is a promising source of anti-leishmanial agents.

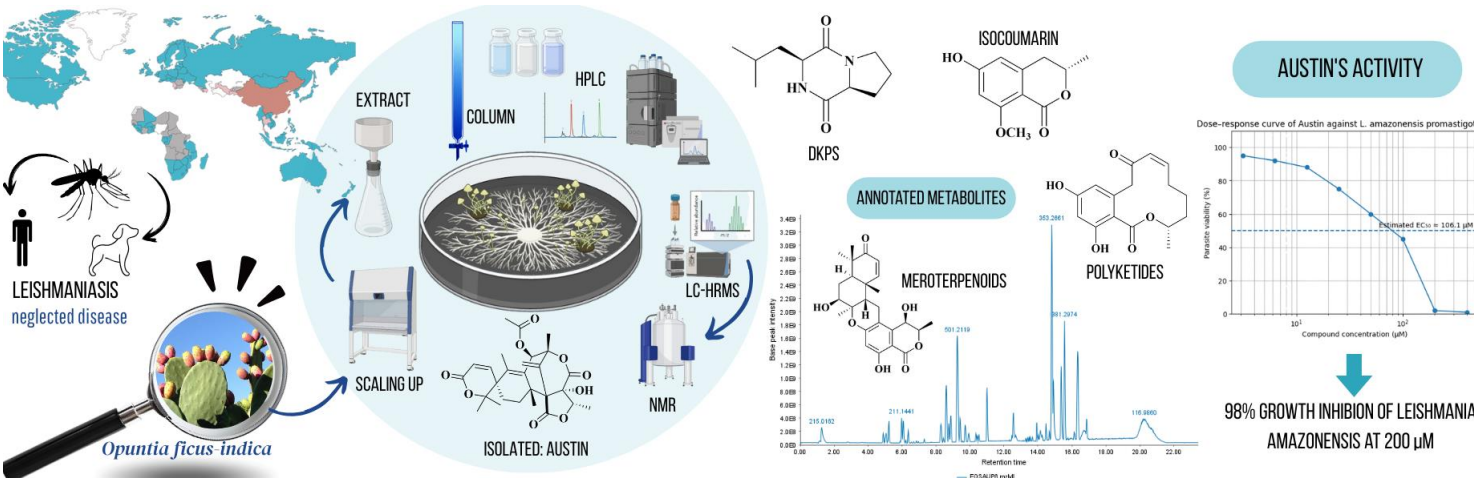
Resumo/Abstract

Leishmaniasis is a neglected parasitic disease of major public health concern, with current treatments limited by toxicity, cost, and resistance [1]. Endophytic fungi, which inhabit plant tissues harmlessly, play an important role in producing bioactive specialized metabolites (SM) [2]. This study provides a comprehensive chemical characterization of the endophytic fungus*Talaromyces*sp. P6 from*Opuntia ficus-indica*, typical of the Semiarid Brazilian Northeast. The metabolite profile of P6 was assessed using UHPLC/ESI-Q-Orbitrap-based metabolomics combined with a dereplication workflow supported by an in-house HRMS database of*Talaromyces*metabolites to guide the discovery of anti-leishmanial metabolites. Among 379 detected features, 23 were annotated (retention time 2.0-11.0 min), revealing the presence of two diketopiperazines, two coumarins, eight meroterpenoids, ten polyketides, and one quinone. Chromatographic fractionation of the ethyl acetate extract obtained from P6 cultivated on potato dextrose agar (PDA) for 7 days at 28 °C led to the isolation of the compound detected at m/z 501.2119 $[M+H]^+$. Structural elucidation based on 1D and 2D NMR analyses identified this compound as the meroterpenoid austin (1). The antiparasitic activity of 1 against*Leishmania amazonensis*MHOM/Br88/Ba-125 promastigotes was evaluated after 72 h using the Alamar Blue viability assay. Austin exhibited an inhibition rate of 98% at 200 µM and an IC_{50} value of 106.1 µM. In cytotoxicity assays against uninfected H9c2 cells, compound 1 presented a CC_{50} value of 351 µM, indicating moderate selectivity. Overall, these findings highlight*Talaromyces*sp. P6 as a promising source of bioactive meroterpenoids and support austin as a potential lead compound for the development of new anti-leishmanial agents.

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Isolation, metabolite annotation and antileishmanial activity of Talaromyces sp. P6

Agradecimentos/Acknowledgments

UFBA, PPGQUIM, CNPq, FAPESB, LaIPHE e LaBioQuiMi

Estudo das características químicas dos compostos bioativos de fitoterápicos da lista do Relação Nacional de Medicamentos Essenciais do SUS

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Palavras Chave:*Caracterização química, Fitoterápicos, RENAME, Compostos Bioativos, Polaridade*

Highlights

The polarity of phenolic compounds, terpenoids, and alkaloids determines the formulations listed in RENAME and guides more accessible dosage methods for the Brazilian Unified Health System (SUS).

Resumo/Abstract

A Relação Nacional de Medicamentos Essenciais (RENAME) é um instrumento estratégico para orientar a seleção e o uso de medicamentos no SUS. No entanto, os fitoterápicos ainda enfrentam desafios relacionados à caracterização química de seus compostos bioativos, devido à complexidade das matrizes vegetais e à semelhança estrutural entre diversos metabólitos. O presente estudo analisa as propriedades químicas dos fitoterápicos do RENAME, correlacionando os grupos funcionais às características hidrofílicas ou hidrofóbicas, com o objetivo de compreender como essas diferenças estruturais determinam solubilidade, justificando os tipos de formulações. As espécies da lista apresentam predomínio de metabólitos fenólicos, seguidos por terpenoides e alcaloides. Compostos fenólicos: incluem ácidos cafeoilquínicos (alcachofra), ácido gálico e derivados (aroeira), taninos (espinheira-santa), cumarina (guaco), isoflavonas (soja), salicina (salgueiro) e antraquinonas glicosiladas como barbaloína (babosa) e cascarosídeos (cáscara-sagrada), apresentando maior polaridade e solubilidade em sistemas hidroalcoólicos. Terpenoides: englobam iridoides (garra-do-diabo) e monoterpenos como mentol e mentona (hortelã piperita), de menor polaridade e, portanto, maior afinidade por sistemas lipofílicos. Alcaloides: os alcaloides oxindólicos pentacíclicos (unha-de-gato) apresentam polaridade moderada e distribuição preferencial em frações menos polares. A polaridade determina o tipo de formulação: espécies polares (ricos em polifenóis ou glicosídeos fenólicos) formam infusões, extratos aquosos e xaropes; espécies de polaridade intermediária (agliconas fenólicas ou alcaloides) dão origem a tinturas e extratos hidroalcoólicos; espécies menos polares (terpenos) são empregadas em pomadas, géis ou cápsulas de extratos secos. A organização química é essencial para desenvolver métodos de doseamento alternativos e acessíveis, devido ao alto custo do HPLC e da CG para farmácias de manipulação.

Agradecimentos/Acknowledgments

FAPEMIG, IQUFU, CAPES, CNPq

Estudo do perfil químico de diferentes espécies de corais após estresse térmico

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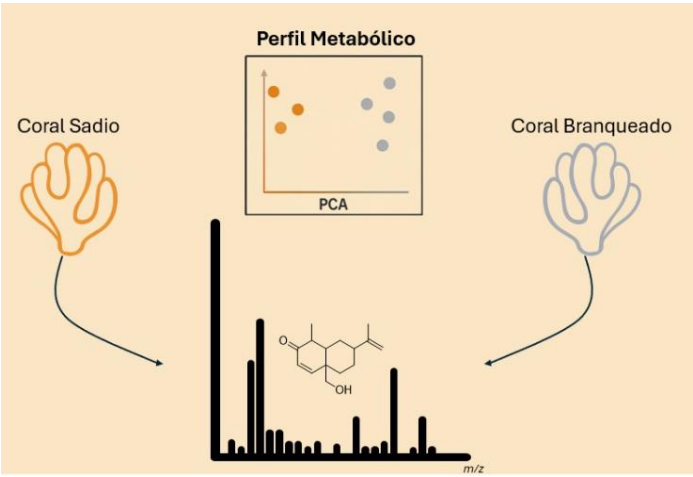
Palavras Chave:*metabolômica,espectrometria de massas,aquecimento global,produtos naturais*

Highlights

Untargeted LC-MS metabolomics was applied to compare healthy and thermal stressed corals, aiming to identify chemical markers associated with coral bleaching.

Resumo/Abstract

Os recifes de corais estão entre os ecossistemas mais biodiversos do planeta e desempenham papel essencial na manutenção da vida marinha, na economia e como fonte de compostos bioativos. Entretanto, esses ecossistemas vêm sofrendo severas ameaças, principalmente devido ao branqueamento de corais, fenômeno associado ao aumento da temperatura dos oceanos causado pelas mudanças climáticas. O branqueamento ocorre quando os corais perdem suas algas simbióticas, resultando em alterações fisiológicas e químicas que podem levar à morte do organismo. Neste contexto, o presente trabalho tem como objetivo avaliar as diferenças no perfil químico de diferentes espécies de corais submetidos a estresse térmico, visando à identificação de possíveis marcadores químicos associados ao branqueamento. Amostras de corais do oceano Atlântico, incluindo Mussismilia hispida, Siderastrea stellata, Madracis decactis, Phyllangia americana, Astrangia rathbuni, Tubastrea coccinea e T. tagusensis foram submetidas a experimentos controlados em aquário, com exposição a diferentes temperaturas e tempos de incubação. Os metabólitos foram extraídos por solventes orgânicos e os extratos analisados por cromatografia líquida acoplada à espectrometria de massas (LC-MS/MS) em abordagem untargeted. Os dados obtidos foram processados por ferramentas de metabolômica e os dados submetidos a análises estatísticas. A identificação dos metabólitos de interesse foi realizada por busca em bibliotecas espectrais, como a plataforma Global Natural Products Social Molecular Networking (GNPS), e por construção de redes moleculares. Foram anotados metabólitos já descritos associados diretamente de corais compostos como Tubastrindole B isolado de corais do gênero Tubastrea, isocarcophytoxide isolados de corais moles, entre outros.



Esquema da metodologia do projeto

Agradecimentos/Acknowledgments

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Estudo do perfil químico e atividade enzimática dos extratos de Lippia origanoides visando aplicação cosmética.

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Palavras Chave:*Lippia origanoides, desreplicação, inibição, tirosinase, elastase.*

Highlights

Ethanolic extracts of*Lippia origanoides*showed promising tyrosinase inhibition, with the DCM fraction reaching 92% at 100 µg/mL; dereplication annotated 15 phenolic compounds driving activity.

Resumo/Abstract

A biodiversidade brasileira é fonte de compostos bioativos aplicáveis à indústria cosmética, especialmente aqueles relacionados à prevenção do envelhecimento cutâneo e de manchas na pele. Este trabalho teve como objetivo avaliar extratos etanólicos de folhas frescas e secas de*Lippia origanoides*Kunth (Verbenaceae) (SisGen A9D0265), visando à caracterização química e à atividade inibitória frente às enzimas tirosinase e elastase. Os extratos foram obtidos por percolação em etanol, fracionados por partição líquido-líquido, cromatografia em coluna e analisados por CLAE-DAD. Os cromatogramas indicaram alta similaridade entre os perfis químicos dos extratos, apesar das diferenças nos métodos de extração. Nos ensaios enzimáticos, extratos e frações não apresentaram atividade relevante frente à elastase. Em contraste, observou-se inibição promissora da tirosinase, com destaque para a fração em diclorometano, que apresentou 92% de inibição a 100 µg/mL. A desreplicação química do extrato etanólico foi realizada por LC-HRMS, nos modos de ionização positivo e negativo, sendo os dados de MS/MS analisados utilizando as plataformas SIRIUS e GNPS. Os compostos anotados foram 5,7-diidroxicumarina (**1**), florizina (**2**), floretina (**3**), eriodictiol glicosilado (**4**), eriodictiol (**5**), luteolina (**6**), quercetina (**7**), quercetina glicosilada (**8**), naringenina (**9**), taxifolina (**10**), acteosídeo (**11**), cirsimaritina (**12**), hesperetina (**13**), luteolina glicosilada (**14**) e apigenina (**15**). Em conjunto, os resultados sugerem que constituintes de média polaridade são os principais responsáveis pela atividade observada e evidenciam o potencial de*L. origanoides*como fonte de ingredientes ativos para aplicações cosméticas.**Referência:**Vieira, J. L. Análise química de*Lippia origanoides*Kunth e prospecção de ativos para potencial uso cosmético. 2025. Dissertação (Mestrado em Química) – Instituto de Química, Universidade Federal de Catalão, Catalão, 2025.

Agradecimentos/Acknowledgments

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Estudo fitoquímico e de cinética de oxidação de polifenóis isolados de alimentos de origem vegetal da dieta dos brasileiros.

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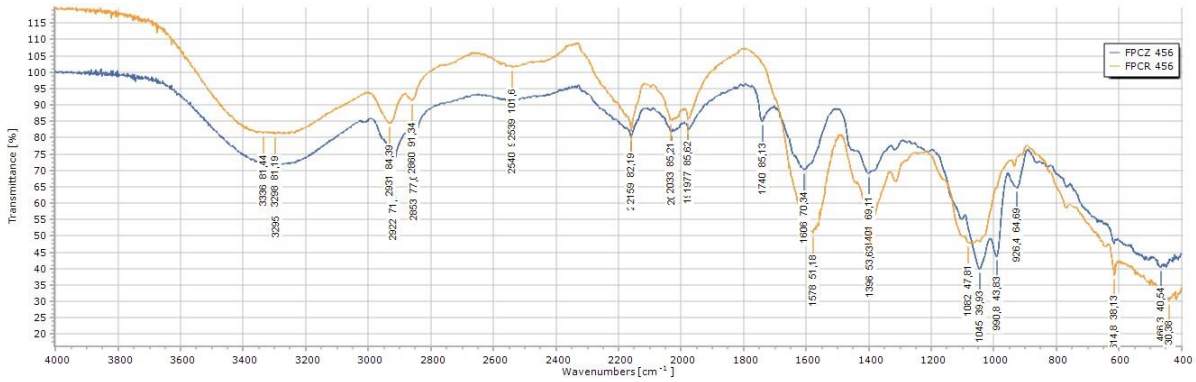
Palavras Chave:*Polifenóis, Dieta brasileira, Antioxidantes, Estudo fitoquímico.,polifenóis,direta brasileira,antioxidantes,estudo fitoquímico*

Highlights

The project studied polyphenols in red and black beans, relating chemical structure and thermal changes. Extraction and chromatography techniques, followed by FTIR showed some heat-induced changes.

Resumo/Abstract

Este projeto teve como objetivo o estudo fitoquímico e a caracterização de polifenóis extraídos de alimentos representativos da dieta brasileira, visando correlacionar a estrutura química desses compostos com a atividade antioxidante e com alterações induzidas pelo processamento térmico. Foram utilizados feijão preto e vermelho, nas formas crua e cozida, como modelos experimentais. A metodologia envolveu revisão bibliográfica, extração sólido-líquido em Soxhlet utilizando solventes de polaridade crescente (hexano, acetona, etanol e água), seguida de fracionamento por cromatografia em coluna de sílica gel da fração etanólica. As frações obtidas foram analisadas por cromatografia em papel, para comparação e agrupamento de frações equivalentes. As frações consolidadas foram concentradas até à secura e caracterizadas por espectroscopia no infravermelho (FTIR). Os espectros revelaram diferenças entre as amostras. No feijão vermelho cozido, as frações mais polares apresentaram banda média e estreita em 1743 cm^{-1}, atribuída ao estiramento de carbonila de cetonas conjugadas, sugerindo a presença de flavonóis, flavonas ou isoflavonas. As frações menos polares não apresentaram variações relevantes entre as amostras crua e cozida, indicando estabilidade térmica desses compostos. Em contraste, as frações menos polares do feijão preto evidenciaram transformações químicas induzidas pelo aquecimento. O feijão cozido apresentou bandas médias e largas de ácidos carboxílicos em 991 e 1045 cm^{-1}, ausentes no feijão cru. As frações polares do feijão preto exibiram uma banda média e estreita em 1977 cm^{-1}, atribuída a vibrações de lactonas ou ésteres complexos, compatível com classes fenólicas como cumarinas ou taninos hidrolisáveis, ausente no feijão cozido o que indica que foram extraídas no cozimento. Esses resultados subsidiam etapas futuras, como identificação por cromatografia acoplada à espectrometria de massas, estudos de cinética de oxidação e avaliação da atividade antioxidante.



Espectro de FTIR das frações menos polares do feijão preto cru (FPCR 456) e cozido (FPCZ 456).

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ESTUDOS DA VARIAÇÃO SAZONAL E CIRCADIANA E DO POTENCIAL ANTI-LEISHMANIA INFANTUM DOS COMPOSTOS VOLÁTEIS DE SCHINUS TEREBINTHIFOLIUS RADDI

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Palavras Chave:*Compostos voláteis, variação sazonal, S.terebinthifolius, antileishmania.*

Highlights

A composição química do óleo essencial de*S.Terebinthifolius*apresentaram estabilidade circadiana e sazonal, com predominância de mono- e sesquiterpenos e atividade*antileishmania.*

Resumo/Abstract

No presente estudo foi analisada a composição química e o potencial anti-***Leishmania infantum***dos óleos essenciais das folhas de***Schinus terebinthifolius***, em quatro diferentes períodos (6h, 12h, 18h e 24h) ao longo de um ano (16º dia dos meses de dezembro/24, março/25, junho/25, setembro/25 e dezembro/25). Após extração por**hidrodestilação**, foram observadas pequenas alterações nos rendimentos dos óleos (de 0,51 a 0,78%). Qualitativamente, os óleos se mostraram constituídos, predominantemente por**a- eb-pinenos e germacrenos B e D**. Sob o aspecto quantitativo, foi observada maior proporção de sesquiterpenos em todos os períodos de coleta, destacando-se os derivados não oxigenados (de 39% as 6h de dezembro/24 a 63% as 24h de setembro/25). No entanto, foi detectada elevada concentração de derivados C_{15} oxigenados no mês de março/2025, que variou entre 21 - 23% (as 06h e 12h) a 12 – 17% (as 18h e 24h), período esse onde foi observada maior precipitação na região de coleta. Nos demais períodos do ano, tais compostos foram detectados em concentrações inferiores a 2%. Quanto aos monoterpenos, maiores concentrações dos mesmos foram observadas nos meses de dezembro de 2024 e 2025 (> 50%) ao passo que nos demais períodos tal proporção foi de aproximadamente 35%. Quando testados contra as formas promastigotas de***L. infantum***, todos os óleos causaram**100% de morte do parasita a 200mg/mL**. Para avaliar os efeitos dos principais compostos na bioatividade, um**pool dos óleos essenciais foi obtido e tal material foi submetido**à**cromatografia em coluna de SiO_2/$AgNO_3$**, fornecendo**α-pineno, β-pineno, α-copaeno, germacreno D e germacreno B**. Esses compostos foram testados individualmente e apresentaram valores de**EC_{50} de 15,5, 12,3, 18,1, 25,6 e 46,5mg/mL**, respectivamente, com baixa toxicidade frente às células**NCTC (CC_{50} > 200mg/mL), sugerindo que os monoterpenos, mais ativos, possam ser, em parte, responsáveis pela ação observada para os óleos brutos**.

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CNPq, FAPESP, CAPES

Evaluation of Antioxidant Activity by UV-Vis of Oils Extracted from Capsicum chinense Cultivars

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Palavras Chave:*DPPH,Antioxidant activity,Capsicum chinense*

Highlights

*Capsicum chinense*oils exhibited high antioxidant activity, with free radical inhibition rates of 90.24% (Maria Bonita) and 90.15% (Biquinho) in the DPPH assay.

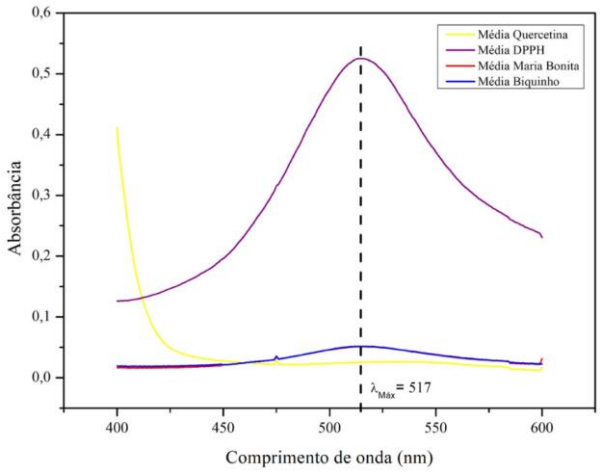
Resumo/Abstract

This study aimed to evaluate the antioxidant activity of oils extracted from peppers of the species*Capsicum chinense*(cultivars Maria Bonita and Biquinho), obtained from the germplasm bank of UFSCar – Araras campus. The methodology was based on the analytes' ability to scavenge DPPH free radicals (2,2-diphenyl-1-picrylhydrazyl).

The oils were obtained from approximately 250 g of plant material subjected to continuous Soxhlet extraction using 500 mL of hexane as solvent. After extraction, the extract was concentrated by rotary evaporation and purified in a separating funnel with three successive washes of 10 mL hexane. The organic phase was dried with anhydrous sodium sulfate, and the oil was kept in an open amber flask under a fume hood for complete solvent evaporation.

Stock solutions containing 4.8 mg of oil from each cultivar were prepared in 50 mL of ethanol. Quercetin was used as a positive control at the same concentration. The DPPH solution was prepared at 2.4 mg per 100 mL of solvent and homogenized, protected from light for 30–60 minutes due to photosensitivity. Samples consisted of 3 mL ethanol, 500 µL of study material, and 300 µL of DPPH solution, with respective controls.

Absorbance readings were performed in triplicate using a UV-Vis spectrophotometer in the 400–600 nm range, with maximum absorption at 517 nm. Data were obtained from triplicate means and analyzed using Origin® software. Oils from Maria Bonita (90.24 ± 2.11%) and Biquinho (90.15 ± 2.12%) showed high free radical inhibition, comparable to quercetin (95.13 ± 1.88%). These results highlight the antioxidant potential of*Capsicum chinense*cultivars for industrial, food, and pharmaceutical applications.
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UV-Vis Absorption Spectra of DPPH Radical Inhibition

Agradecimentos/Acknowledgments

CNPq, CAPES, FAPESP

"Evaluation of plant extracts for the selection of potential xanthine oxidase inhibitors"

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Palavras Chave:*Enzymatic inhibition,polyamide,tannins,solid-phase extraction,Banisteriopsis caapi*

Highlights

33% of the mass of the crude*Banisteriopsis caapi*extract was removed by cleaning with polyamide, maintaining inhibitory activity.

Resumo/Abstract

One of the strategies used for drug discovery is the search for inhibitors of therapeutic targets, such as xanthine oxidase (XO) inhibitors. XO is the terminal enzyme of purine catabolism in humans, catalyzing the oxidation of hypoxanthine to xanthine and finally to uric acid. Its clinical relevance is evident in neurodegenerative, oncological, immunological, and inflammatory pathologies. This study aimed to identify the most promising samples with xanthine oxidase (XO) inhibitory activity among five pre-selected plant species:*Lantana camara*(Lc),*Stachytarpheta jamaicensis*(Sj),*Acmella oleracea*(Ao),*Banisteriopsis caapi*(Bc), and*Ageratum conyzoides*(Ac). The plants were oven-dried (40 °C), pulverized, and subjected to extraction with ethanol:water (70:30). The crude extracts were concentrated under vacuum and fractionated by liquid-liquid partitioning with a polarity gradient (hexane, ethyl acetate, and butanol). To avoid false-positive results, tannins were removed using polyamide solid-phase cartridges. This step was necessary because enzymatic precipitation by tannins reduces the amount of the catalytic product (uric acid). The inhibitory activity of the extracts and fractions was determined using the enzyme in solution and quantifying the uric acid produced by HPLC at 290 nm. The yields obtained from the crude extracts of Lc, Sj, Ao, Bc, and Ac were 28.8%, 31.5%, 32.3%, 25.9%, and 31.2%, respectively. The results of the enzymatic inhibition highlighted the need to use polyamide to remove tannins, as its non-elimination led to overestimated results. The crude extract of*B. caapi*showed the best results in inhibiting XO (12.8% after tannin removal), and its fractionation indicated the best inhibitory activity of the butanolic fraction (55% inhibition) (Fig. 1). These results suggest the potential use of the butanolic fraction of*B. caapi*for future studies.

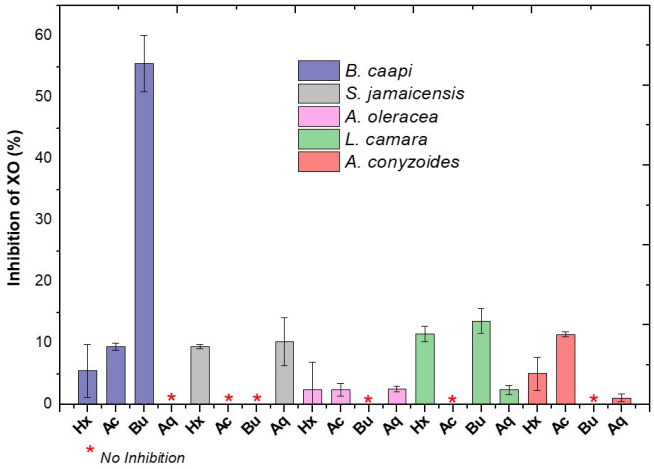


Fig.1 Xanthine oxidase inhibition (%) obtained for fractions of plant species Ac, Lc, So, Sj, and Bc

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Exploring the metabolic diversity of Tetragonisca angustula-associated Actinomycetota in the search for antimicrobial compounds.

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Palavras Chave:*Stingless bees,Actinomycetota,Bioactive Metabolites,Natural Products*

Highlights

Actinomycetota isolated from*Tetragonisca angustula;*Eight strains exhibited activity against bee/human pathogens; Unassigned MS peaks suggest the presence of novel compounds in the active fractions.

Resumo/Abstract

Stingless bees play an essential role in the pollination of the native flora of tropical countries. These bees may establish complex symbiotic interactions with diverse microbial communities, which perform fundamental roles in the hive and synthesize specialized metabolites that mediate defensive symbiosis. Beyond their ecological role, these metabolites can also exhibit inhibitory potential against human pathogens, highlighting these microbial communities as a promising source in the research of novel natural products. This work aimed to isolate and identify the Actinomycetota associated with*Tetragonisca angustula*(Jataí) to evaluate the antimicrobial potential of its metabolites. The sampling was conducted at a colony maintained in the meliponary of the FFCLRP-USP. The bacterial strains were isolated from nurse bees using a chitin-based solid medium and the isolates were tested for antimicrobial activity against pathogenic microorganisms. Within the 22 isolates, 42% demonstrated inhibitory potential, with some showing a generalist activity, while others were more selective against specific pathogens. Inhibitory activity was observed for*P. larvae*and the entomopathogenic fungi*B. bassiana*and*M. anisopliae*, as well as the human pathogens*C. albicans*and*S. aureus*. The 16S rRNA sequencing and phylogenetic analysis of the active strains led to the identification of Micromonospora and Streptomyces genera. Crude extracts from the isolates were obtained and bioactivity-guided fractionation using solid-phase extraction ($MeOH/H_2O$) and HPLC-DAD-ELSD analysis allowed the selection of the most promising fractions. Mass spectrometry analysis of the active fractions revealed several unassigned peaks suggesting the possibility of novel bioactive compounds, including a possible new analog of madurastatin. The isolation and characterization of these metabolites are currently underway to further elucidate the metabolites involved in the Jataí bee microbiome interactions.

Agradecimentos/Acknowledgments

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Fingerprint de canabinoides em inflorescências de Cannabis sativa L. obtidas de clones in vitro: comparação entre clones por CLAE–DAD–EMAR/EMAR

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Palavras Chave:*Cannabis sativa,Fingerprint,Micropropagação*

Highlights

Fingerprint de inflorescências de*Cannabis*por CLAE–DAD–EMAR

Comparação de extratos etanólicos de clones obtidos por micropropagação*in vitro*e por estaquia

Resumo/Abstract

Em fármacos à base de*Cannabis sativa*, a homogeneidade genética é frequentemente utilizada como critério de padronização, sob a premissa de que clones produzirão perfis químicos equivalentes. No entanto, o perfil de metabólitos pode sofrer variações em função do método de clonagem e pelo cultivo. Descrevemos a análise de inflorescências femininas obtidas a partir de clones do genótipo 216, inicialmente estabelecidos*in vitro*(LabCultive - UFG), aclimatizados e cultivados*ex vitro*. As sementes e o material propagativo foram cedidos pela Associação Curando Ivo (Goiás, Brasil), amparados por*habeas corpus*preventivo (Processo: 1000888-59.2020.4.01.3500/5ª Vara Federal Criminal da SJGO). Foram analisados os extratos etanólicos da planta micropropagada (216_A), e de seu respectivo clone obtido por estaquia (216_B), cujos rendimentos médios foram de 11,14% para 216_A e 8,38% para 216_B. O perfil químico foi obtido por CLAE–DAD, acoplada a um espectrômetro de massas Q-Exactive (H-ESI). Para o genótipo 216, observou-se no TIC que o íon base principal é o $[M-H]^-$ m/z 357,2071. Outras espécies químicas contribuíram para o fingerprint, como os íons $[M-H]^-$ m/z 359,2232 e $[M-H]^-$ m/z 329,1762. A identificação e quantificação dos principais canabinoides, como o tetrahidrocanabiol (THC) e canabidiol (CBD), compõem a próxima etapa do estudo, e estas análises serão ampliadas para quatro genótipos adicionais, a fim de avaliar a robustez do padrão de canabinoides frente aos processos de clonagem.

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From chemical profile to antitumor activity: a study by ^{1}H NMR and flow cytometry of the hexane extract of the macroalga Dichotomaria huismanii

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Palavras Chave:*Natural products,Secondary metabolites,Bioactive lipids*

Highlights

The hexane extract ofDichotomaria huismanii, at a concentration of 25 µg/mL, induces apoptosis (85.3 ± 0.2%) in THP-1 cells, with low induction of necrosis (4.9 ± 0.1%).

Resumo/Abstract

*Dichotomaria huismanii*is a marine macroalga found along the northeastern coast of Brazil with a chemical and biological profile that is still poorly explored. Studies with extracts of different polarities indicate that this species exhibits antimicrobial, cytotoxic, and antioxidant activities. In this context, the present study aimed to perform the chemical characterization and evaluate the antitumor activity of the hexane extract of this macroalga.The material, collected at Praia do Forte, Mata de São João, Bahia, was ground, subjected to ultrasound-assisted extraction with hexane, and the obtained extract was characterized by proton nuclear magnetic resonance (^{1}H NMR, 500 MHz). The antitumor activity was evaluated in THP-1 lineage cells treated with the extract at concentrations of 50 and 25 µg/mL for 48 hours and analyzed by flow cytometry with Annexin V-FITC and propidium iodide.The ^{1}H NMR analysis showed a predominance of signals in the aliphatic region (δ 0.8–2.5 ppm), indicating mainly the presence of fatty acids, neutral lipids, and aliphatic terpenoids, a profile similar to that described for macroalgae of the family Galaxauraceae, such as*Galaxaura rugosa*.In the evaluation of the antitumor effect, the concentration of 50 µg/mL resulted in 87.3 ± 0.2% apoptosis and 2.3 ± 0.1% necrosis. At the concentration of 25 µg/mL, maintenance of apoptosis was observed (85.3 ± 0.2%) with an increase in necrosis to 4.9 ± 0.1%. The high induction of apoptosis in THP-1 cells may be associated with lipophilic metabolites, described as interacting with cell membranes and modulating programmed cell death pathways.Studies with species from the same family report terpenoids with antitumor activity, suggesting that similar metabolites contribute to the observed effect. The fractionation of the extract and biological evaluation of the major constituents are in progress to confirm the antitumor potential of*Dichotomaria huismanii*.

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Geopropolis from Melipona quadrifasciata anthidioides as a source of bioactive isoflavonoids: isolation and biological activity of vestitol

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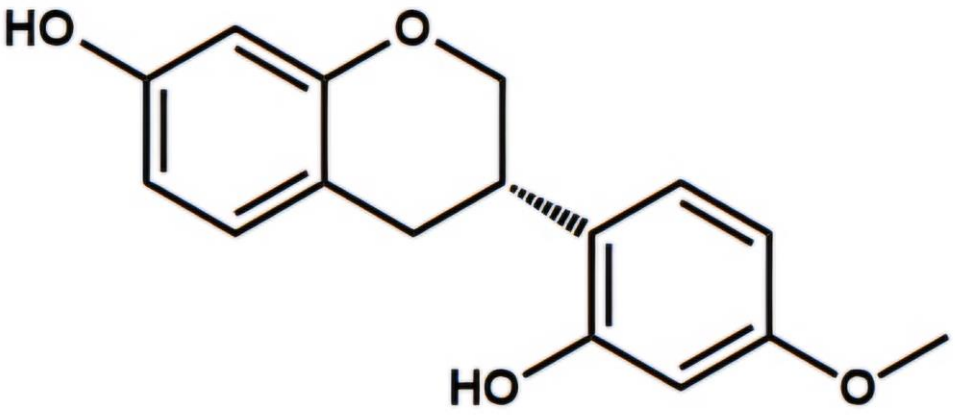
Palavras Chave:*Geopropolis, vestitol, isoflavonoids, antifungal and antiparasitic activity*

Highlights

Isolation and characterization of isoflavonoids from geopropolis of*Melipona quadrifasciata anthidioides*. Antifungal and antiparasitic evaluation of isolated vestitol.

Resumo/Abstract

Geopropolis is a resinous material produced by stingless bees from a mixture of plant resins with soil and/or clay, playing an essential role in protecting the hive against pathogenic microorganisms. This biological potential has motivated studies focused on the prospection of bioactive specialized metabolites. Among the targets of interest are clinically relevant fungi, such as*Sporothrix brasiliensis*, the main etiological agent of sporotrichosis in Brazil, and*Candida albicans*, classified as a critical priority fungal pathogen by the World Health Organization, as well as the protozoan*Trypanosoma cruzi*, the causative agent of Chagas disease. In this study, geopropolis from the mandaçaia bee (*Melipona quadrifasciata anthidioides*), collected at Bosque da Barra (RJ), was investigated aiming at the isolation, identification, and biological evaluation of its chemical constituents. From 10 g of geopropolis, an ethanolic extract (EEGP-M) was obtained and subjected to liquid–liquid partitioning, yielding hexane, dichloromethane and hydroalcoholic fractions. The dichloromethane fraction exhibited antifungal activity, with MIC values of 562 µg·mL^{-1} against*S. brasiliensis*and*C. albicans*, and was selected for chromatographic fractionation. Vestitol, medicarpin, isoliquiritigenin, and formononetin were isolated, bioactive compounds previously reported in red propolis. Vestitol, obtained in higher yield and high purity (95%, HPLC-DAD), showed superior antifungal activity compared to the dichloromethane fraction, with MIC values of 170 µg·mL^{-1} against*S. brasiliensis*and 340 µg·mL^{-1} against*C. albicans*, in addition to expressive antiparasitic activity against*T. cruzi*(IC_{50} = 35.13 µM). These results highlight geopropolis as a promising natural matrix for obtaining bioactive specialized metabolites, emphasizing vestitol as an isoflavonoid of interest in the context of Natural Products Chemistry.



Vestitol isolated from geopropolis of the mandaçaia bee

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Halogenated Alkaloids from the Bryozoan Amathia brasiliensis

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Palavras Chave:*Marine natural products;,secondary metabolites;,marine invertebrates;,spectroscopic analysis;,isolation*

Highlights

Six new alkaloids, cebimarins A–F, were isolated from the organic extract of A. brasiliensis. Structures and absolute configurations were determined by spectroscopic data and ECD.

Resumo/Abstract

Bryozoans are recognized as a prolific source of structurally unique secondary metabolites with relevant pharmacological potential. Species belonging the genus*Amathia*attracted considerable attention due to the presence of bioactive indole alkaloids, particularly halogenated derivatives. In this report, the organic extract of*Amathia brasiliensis*, collected off the coast of São Sebastião, São Paulo State, Brazil, was chemically investigated. Lyophilized specimens were exhaustively extracted with MeOH, followed by liquid–liquid partitioning and systematic chromatographic fractionation using solid-phase extraction and reversed-phase high-performance liquid chromatography. Chemical profiles of the resulting fractions were monitored by HPLC coupled to UV and mass spectrometry detection, enabling the targeted isolation of alkaloid-rich fractions. Six previously undescribed indole alkaloids were isolated and named as cebimarins A–F. These compounds were identified as the major constituents of fractions that exhibited antimalarial activity. High-resolution mass spectrometry and complementary spectroscopic analyses confirmed the presence of halogenated scaffolds, including both brominated and mixed brominated/chlorinated derivatives. The discovery of six new halogenated indole alkaloids establishes*A. brasiliensis*as a prolific and unexplored source of marine natural products and reinforces the relevance of Brazilian bryozoans in the search for novel bioactive molecules with potential antimalarial applications.

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High-Resolution Ion Mobility Spectrometry-Mass Spectrometry Analysis of Parotoid Gland Secretions from Bufonid Species

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Palavras Chave:*Bufadienolides,Parotoid Secretions,TIMS,Ion Mobility,Metabolomics*

Highlights

High-Resolution IMS-MS of Toad Parotoid Secretions; TIMS-MS profiling of bufadienolide-rich toad secretions

Resumo/Abstract

Bufadienolides are the main cardiotonic steroids present in the parotoid gland secretions of Bufonidae toads and exhibit antitumor, antimicrobial, and antiparasitic activities [1]. Their analysis is challenging due to extensive isomerism and variable ionization efficiencies [2]. This study applies ion mobility spectrometry–mass spectrometry (TIMS-MS) for metabolomic profiling of bufadienolide-rich parotoid secretions from four Bufonidae species:*Peltophryne fustiger*,*Peltophryne florentinoi*,*Peltophryne peltocephala*from Cuba, and*Rhinella ornata*from PETAR, Brazil. Metabolomic studies of parotoid secretions from Cuban endemic toads remain scarce, with only one previous report describing bufadienolides from*P. fustiger*[3]. Secretions from five individuals per species were collected by gentle mechanical compression, extracted with methanol (ultrasonication, three cycles), centrifuged (4 °C, 12,000 rpm), dried, and reconstituted in acetonitrile/water (50:50 (v/v), 0.1% formic acid). Samples (500 µg/mL) were injected (4 µL) and analyzed using a Bruker timsTOF fleX instrument with ESI in positive ion mode. TIMS parameters included N_2 dry gas at 10 L/min, 100 ms accumulation time, a 400 ms ramp time, and a $1/K_0$ range of 0.45–1.45 Vs/cm². PASEF MS/MS experiments employed two collision energy ramps (30–50 eV for diagnostic neutral losses and 50–70 eV for deeper bufotoxin fragmentation). Hydrocortisone (1 µg/mL) was used as an internal standard. Data were processed using DataAnalysis 5.0 and MetaboScape. A total of 25 bufadienolides and bufotoxins were detected and characterized, including five putative novel isomers resolved by collision cross section values (196–652 Å²). Species-specific models are under development. Overall, this TIMS-MS workflow highlights the potential of ion mobility for isomer-selective profiling of steroid-rich secretion.
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HPLC-QTOF-MS–Based Chemical Profiling of Anti-Inflammatory Specialized Metabolites from Endophytic Fungal Co-Cultures

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Palavras Chave:*Endophytic fungi,HPLC-QTOF-MS,Fungal co-culture,Metabolomic profiling,Anti-inflammatory*

Highlights

Endophytic fungal co-culture activated silent pathways, increased metabolite diversity, and yielded extracts with potent dual COX and LOX inhibitory activity.

Resumo/Abstract

The discovery of bioactive molecules for drug development has historically relied on the exploration of natural resource, often involving extractive approaches that require large amounts of plant biomass. Such practices threaten biodiversity, particularly in endangered biomes such as the Atlantic Forest. In this context, microbial chemistry has emerged as a sustainable alternative. Endophytic fungi, which inhabit internal plant tissues without causing apparent harm, represent a renewable source of structurally diverse specialized metabolites. Once isolated, endophytes can be readily cultivated under laboratory conditions, enabling continuous metabolite production while preserving the host plant.*Ocotea*sp. have a long history of ethnopharmacological use in South American traditional medicine, particularly for the treatment of inflammatory conditions. Moreover, endophyte co-culture has proven to be an effective strategy for activating silent biosynthetic pathways, inducing the production of same bioactive metabolites that their hosts. In this study, we investigated the chemical profiles and anti-inflammatory potential of crude extracts of the endophytic fungi*Lasiodiplodia*sp. and*Lentinus*sp., isolated from*Ocotea diospyrifolia*. Single and dual cultures were grown on PDA (Potato Dextrose Agar) for 7 days at 28°C. Ethyl acetate extracts were analyzed by HPLC-QTOF-MS/MS for metabolic characterization and subjected to in vitro assays to evaluate Cyclooxygenase (COX) and Lipoxygenase (LOX) inhibitory activities.

Comparative metabolomic analysis revealed that co-culture significantly upregulated the production of Perseal G, Asaricin, and*trans*-Asarone. Notably, the extracts exhibited potent dual inhibition of COX and LOX, critical enzymes in the arachidonic acid cascade. These findings validate fungal co-culture as a robust biotechnological strategy for enhancing chemical diversity and accelerating the discovery of novel anti-inflammatory agents.

HRMS analysis of methanol extracts of the leaves of several Psychotria viridis, ingredient of the Ayahuasca brew

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Palavras Chave:*N-dimethyltryptamine Phenolic compounds; Phytochemistry; Mass Spectrometry,Metabolite Profilling.,N,N-dimethyltryptamine,Phenolic compounds*

Highlights

Psychotria viridis is an important source not only of N,N-Dimtheyltriptamine, but also of potentially bioactive proanthocyanidins, which are still poorly explored.

Resumo/Abstract

A great variety of bioactive natural products has been reported for different*Psychotria*species (Rubiaceae). Among the numerous species native to South America,*P. viridis*Ruiz & Pav. (*Chacrona, Rainha,*popular names) has amassed a large interest due its use in the ritualistic brew "*Ayahuasca*" by various indigenous ethnicities and other traditional communities. Recently, the brew has also been consumed in urban rituals in multiple continents. This species is widely recognized for its richness in the indole alkaloid N, N-dimethyltryptamine (DMT). However, there are low reports in the current literature about the phytochemical composition of the phenolic compounds from*P. viridis*, a gap this research seeks to evaluate. For this purpose, we did a targeted HRMS metabolite profiling, as well as identification of the main metabolites in the extracts of the different*P. viridis*accessions focusing on the putative identification of phenolic compounds, mainly flavonoids and proanthocyanidins. Methanol extracts from leaves of twenty-two*P. viridis*cultivated accessions mostly collected in Goiás, Brazil, were analyzed through HRMS direct injection, with positive and negative EsI. With this data, it was possible to detect the presence of DMT and hydroxyl derivative (bufotenine or psylocine) in EsI positive in the 22 samples analysed. In turn, different phenolic compounds, such as trimers of proanthocyanidins and flavonoids heterosides were putative identified in various extracts. In this sense, the negative HRMS EsI analysis were very important for these identifications. Further research is necessary to obtain quantification data to corroborate if the content of classes such as flavonoids and proanthocyanidins is significant, which could be followed by antioxidant and enzyme inhibition assays to explore the bioactive potency and possible therapeutic potential of this phenolic compounds alongside the already recognized presence of DMT.

Agradecimentos/Acknowledgments

Agradecemos aos projetos FAPDF AgroLearning 00193-00002399/2023-10 e Demanda Espontânea 00193-00002220/2023-16.

Identification and behavioral activity of a candidate sex pheromone in Diceraeus melacanthus (Hemiptera: Pentatomidae)

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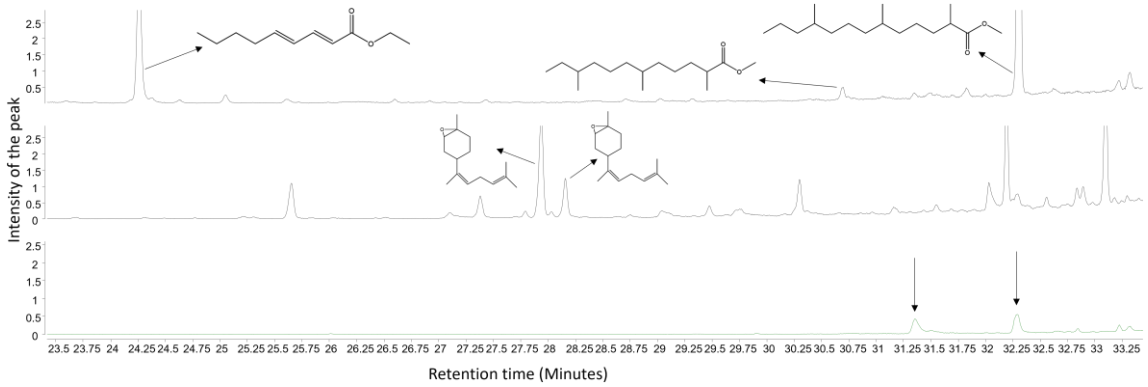
Palavras Chave:*pheromones, pest management, neotropical stink bug, sesquiterpene*

Highlights

Male-specific compounds in the aedeagus reveal a new female-attracting pheromone in the soybean pest*Diceraeus melacanthus*

Resumo/Abstract

Diceraeus melacanthus(Hemiptera: Pentatomidae) is an important pest of soybean and maize crops in Brazil. Its management currently depends on insecticide applications, raising concerns about environmental sustainability. This study aimed to identify potential sex or aggregation pheromones in*D. melacanthus*as a basis for developing more sustainable tools for integrated pest management. Volatiles were collected from both males and females using an air-entrainment system. Additionally, the aedeagus of ten males were dissected and soaked in hexane for five minutes (N = 10). For comparative purposes, aedeagus extracts were also obtained from two other stink bug species,*Euschistus heros*and*Nezara viridula*. All volatile and aedeagus extracts were analyzed by GC-FID and GC-MS. Volatile samples from male and female*D. melacanthus*did not show the presence of sex-specific compounds. However, chemical analysis of the aedeagus extracts from all three species showed the presence of male-specific compounds. In*E. heros*and*N. viridula*, known male sex pheromones previously described in the literature were confirmed. In*D. melacanthus*, two male-specific compounds were identified in the aedeagus extracts: one sesquiterpene and one methyl ester. To confirm the structure, the compound was synthesized, and the retention time and mass spectra of the synthetic compound matched those of the natural product detected in male extracts, confirming its identity. Behavioural assays using a Y-tube olfactometer were conducted with synthetic solutions of the compound. Female*D. melacanthus*showed significant attraction to the arm containing the synthetic compound at doses of 0.02 µg and 0.2 µg (χ^2 = 7.4,*P*= 0.006; χ^2 = 7.8,*P*= 0.005, respectively), whereas males did not exhibit any preference. Further studies are underway to determine the absolute configuration of the identified sesquiterpene and to assess the behavioural activity of the methyl ester.



GC-MS aedeagus extracts (A)E.heros (B)N.viridula (C)D.melacanthus → red arrow: male-only terpene

Agradecimentos/Acknowledgments

This work was financially supported by the National Council for Scientific and Technological Development (CNPq), the Federal District Research Support Foundation (FAP-DF), and the Brazilian Agricultural Research Corporation (EMBRAPA).

Identification and quantification of flavonoids from the leaves of Miconia albicans (Melastomataceae) by UPLC-MS/MS

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Palavras Chave:*Miconia albicans,Flavonoids,LC-MS/MS,Solvent mixture design,Quercetin derivatives*

Highlights

Ternary solvent mixture enhanced flavonoid extraction from*Miconia albicans*leaves, identified by UPLC-ESI-Q-TOF-MS/MS, highlighting quercetin derivatives and ellagic acid.

Resumo/Abstract

Flavonoids are secondary metabolites of great medicinal importance due to various pharmacological effects reported in the literature, such as antioxidant, anti-inflammatory, and antibacterial effects, among others. These substances are found in the leaves of*Miconia albicans*(Melastomataceae), a medicinal plant known as "*canela-de-velho*" (old man's cinnamon), which is popularly used to treat joint pain. The objective of this work is to identify and quantify the flavonoids present in methanolic fractions of different extracts from*Miconia albicans*leaves using LC-MS analysis. The extracts were prepared from 12g of previously dried and ground plant material under extractive compositions delimited by a simplex-centroid design with ethanol, ethyl acetate, dichloromethane, and hexane. The methanolic fractions of these extracts were subjected to reverse-phase analysis by UPLC-ESI-Q-TOF-MS/MS in negative mode for separation and identification of constituents and subsequent quantification of flavonoids using an analytical curve prepared with rutin as an external standard. Of a total of fifteen extractive compositions, six exhibited a chemical profile rich in flavonoids, with the ethanol:dichloromethane:hexane (EDH) composition in a 1:1:1 ratio standing out. MS/MS fragmentation data identified mainly glycosylated flavonols derived from quercetin and kaempferol with different glycosylations, including galloyl groups. Among the major ones, quercetin-galloyl-hexoside (*m/z*615) and quercetin-rhamnoside (*m/z*447) stand out. Furthermore, a high concentration of ellagic acid was found in several extracts. This work shows that a ternary extractive composition was able to provide a higher concentration of flavonoids compared to the ethanolic extract, indicating that solvent mixtures have great potential for future studies.

Agradecimentos/Acknowledgments

I thank the Chemical Sciences Laboratory of UENF and the funding agencies CAPES and FAPERJ.

Identification of Volatile Secondary Metabolites during the Fusarium pernambucanum–Citrus sinensis Interaction

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Palavras Chave:*Citrus,Fusarium,Volatile Compounds,Interaction*

Highlights

In this study, we identified several VOCs, particularly sesquiterpenes, produced during the*F. pernambucanum–Citrus sinensis*interaction using SPME extraction and GC×GC–TOFMS analysis.

Resumo/Abstract

Under climate change scenarios, citrus plants are continuously exposed to phytopathogens of the genus*Fusarium*(1), and insect vectors (2). Phytopathogenic fungi produce volatile organic compounds (VOCs) that modulate interactions with host plants, other microorganisms, and insects (3), potentially facilitating fungal penetration, suppressing plant defenses, and influencing vector attraction for spore dissemination (4). In addition, some VOCs are toxic to plants, while plants have evolved mechanisms to recognize and mitigate these attacks (5). In this study,*F. pernambucanum*was isolated from symptomatic tissues of*C. sinensis*showing rot-like symptoms, as well as from eggs and nymphs of A. woglumi (citrus blackfly) collected from a citrus orchard in northeastern Brazil. To investigate volatile metabolites produced in the host-pathogen interaction,*C. sinensis*plants in vitro were inoculated with the fungus for 14 days. VOCs production profile was evaluated using solid-phase microextraction (SPME) coupled with comprehensive two-dimensional gas chromatography combined with quadrupole time-of-flight mass spectrometry (GC×GC–TOFMS). The results revealed that both control (healthy) plants and plants inoculated with*F. pernambucanum*exhibited a wide diversity of metabolites, belonging to classes such as hydrocarbons, alcohols, and esters. The major VOCs produced during the interaction belonged to the sesquiterpene class, including bicyclogermacrene, muurolene, cadinene, copaene, cuprene, longifolene, among others. Longifolene is produced by some phytopathogenic fungi and can act as an attractant for insects, favoring fungal colonization (6). In addition, monoterpenes such as limonene were significantly more abundant in inoculated samples. These findings provide new insights into the metabolites involved in the response of*C. sinensis*to*F. pernambucanum*infection and deepen the understanding of the fungal biosynthetic machinery involved in terpene production.

Agradecimentos/Acknowledgments

Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), e à Fundação de Amparo à Pesquisa de São Paulo (FAPESP).

Indole alkaloids from Anadenanthera spp.: from ethnobotany to translational pharmacology of tryptamines – A review

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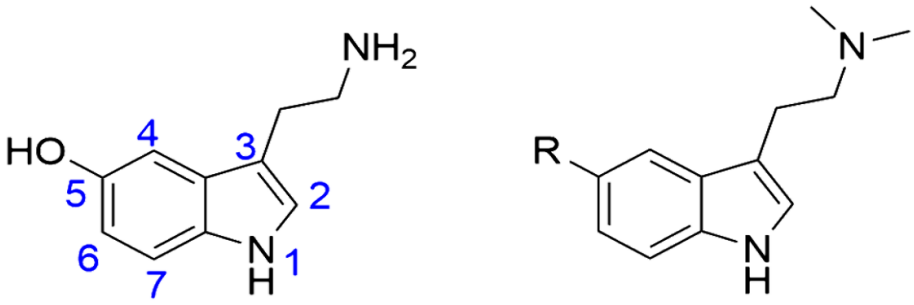
Palavras Chave:*Anadenanthera spp.; Angico; indolic alkaloids; tryptamines; potential antidepressant.*

Highlights

*Anadenanthera*spp. show ethnopharmacological relevance; Indole alkaloids and tryptamines prevail; Rapid antidepressant effects via 5-HT receptors.

Resumo/Abstract

Species of the genus*Anadenanthera*(Angico) are widely distributed in the Brazilian Cerrado and exhibit high ethnopharmacological relevance, with documented use in Indigenous rituals throughout South and Central America, particularly in the form of snuffs. This narrative review aims to integrate ethnobotanical, phytochemical, and pharmacological aspects of*Anadenanthera*species, with emphasis on their historical use by ancestral peoples; the occurrence and distribution of indole alkaloids (Figure 1); and their translational relevance for neuropsychiatric disorders such as depression and anxiety. To this end, a bibliographic search was conducted in indexed databases (SciFinder, PubMed, ScienceDirect, and SciELO), together with Google Scholar and the JANE platform, using combinations of descriptors and boolean operators to systematize three thematic axes: (1) ethnobotanical and morphological characterization of the species; (2) phytochemical profiling of indole alkaloids present in different tissues of Anadenanthera spp. and in snuffs; and (3) pharmacological evidence from preclinical and clinical studies evaluating tryptamines as rapid-acting antidepressant agents. The results indicate that, beyond the broad spectrum of biological activities exhibited by*Anadenanthera*species (e.g. anti-inflammatory, antifungal, and wound-healing), some of the indole alkaloids present in their composition (i.e., bufotenine,*N,N*-dimethyltryptamine [DMT], and 5-methoxy-DMT [5-MeO-DMT]) stand out for their antidepressant potential, with mechanistic evidence supporting agonist activity at 5-HT2A and 5-HT1A receptors due to their structural similarity to the neurotransmitter serotonin (5-HT). Collectively, these findings identify*Anadenanthera*indole alkaloids as translational candidates that bridge traditional knowledge and modern neuropsychopharmacology, offering promising perspectives to inspire the development of new therapeutic strategies in the field of mental health.



Serotonina (5-HT)

R = H (DMT)
R = OH (Bufotenina)
R = MeO (5-MeO-DMT)

Chemical structures of the neurotransmitter serotonin and alkaloids from Anadenanthera spp.

Integrated metabolomic, chemometric, and bioactivity assessment of stems from Banisteriopsis species (Malpighiaceae)

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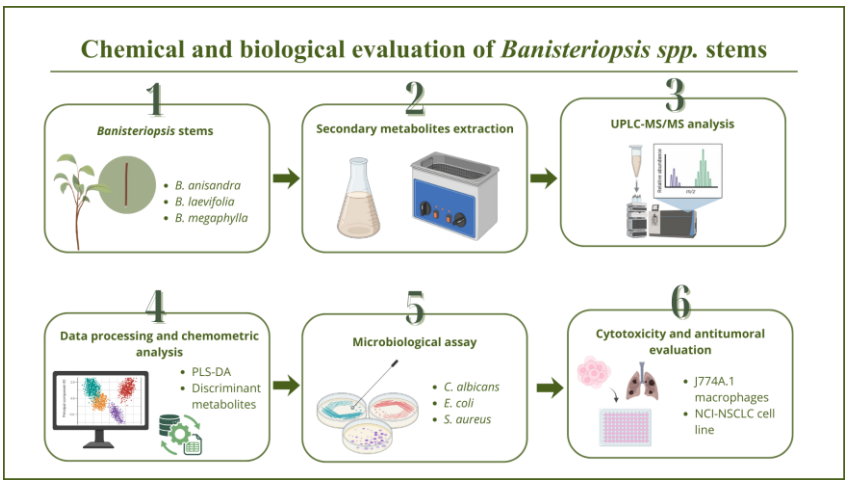
Palavras Chave:*UPLC-MS/MS, PLS-DA, Antifungal, Antibacterial, Cytotoxicity,UPLC-MS/MS,PLS-DA,Antifungal,Antibacterial,Cytotoxicity*

Highlights

Pioneering study on the biological potential of three species of*Banisteriopsis*stems integrating UPLC-MS/MS analysis, chemometrics and biological assays.

Resumo/Abstract

The Malpighiaceae family is recognized for its chemical and biological potential, with studies reporting secondary metabolites exhibitingantioxidant and larvicidal activities, as well as functional properties. However, the stems of these species remain chemically underexplored, which limits their therapeutic potential. This gap is particularly evident in the genus*Banisteriopsis*, where the stem phytochemical profile is still poorly characterized. This study investigated the metabolic profile and biological potential of stems from*B. anisandra*,*B. laevifolia*, and*B. megaphylla*using*untargeted*metabolomic analysis by ultra-high performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS), chemometrics, and bioassays. Partial least squares-discriminant analysis (PLS-DA) revealed that the chemical discrimination among the species is primarily driven by glycosylated quercetins. In microbiological assays, the extracts exhibited antifungal activity against*Candida albicans*(ATCC 10231), with minimum inhibitory concentrations (MICs) of 2000 µg mL^{-1} (*B. anisandra*and*B. laevifolia*) and 1000 µg mL^{-1} (*B. megaphylla*), and a minimum fungicidal concentration (MFC) of 2000 µg mL^{-1} for all three species. Additionally, bacteriostatic activity was observed against*Escherichia coli*(ATCC 25922) and*Staphylococcus aureus*(ATCC 25925) at 2000 µg mL^{-1}. Cytotoxicity assays in J774A.1 macrophages and antitumor assays in the NCI-NSCLC cell line are currently underway to assess cell viability. Overall, these findings highlight Banisteriopsis stems as a promising and previously neglected source of bioactive metabolites, reinforcing their potential for future pharmacological and biotechnological applications.



Experimental workflow for the chemical and biological evaluation of Banisteriopsis spp. stems.

Agradecimentos/Acknowledgments

The author thanks the State University of Londrina (UEL), the Graduate Program in Chemistry (PPGQ/UEL), the laboratories involved, and EMBRAPA for institutional support, infrastructure, technical assistance and collaboration throughout this research.

Integration and Multivariate Analysis of Chemical Compounds and Botanical Characteristics in Brazilian Plants (MPH Collection)

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Palavras Chave:*Brazilian Biodiversity,metabolomics,natural products,multivariate analysis,drug discovery*

Highlights

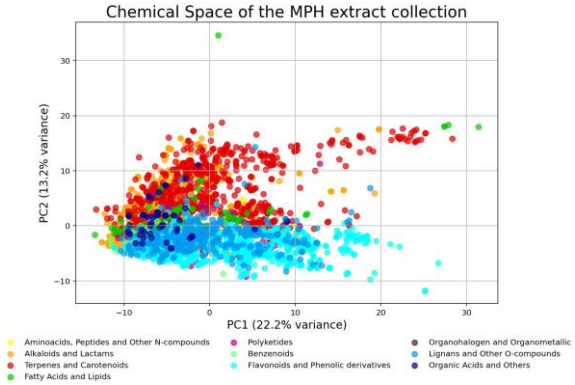
Metabolomics revealed 11,815 compounds with nonredundant high novelty.

Ten chemical superclasses define a broad chemical space.

Biogeographic and botanical patterns shape metabolite distribution.

Resumo/Abstract

Brazilian biodiversity, which contains nearly 20% of the world's species, represents a strategic resource for the bioprospecting of new drugs, particularly given that ~67% of low-molecular-weight pharmaceuticals originate from or are inspired by natural products. This study applied metabolomics and multivariate analyses to correlate chemical, biogeographical, and botanical data from 652 organic plant extracts from Brazilian biodiversity belonging to the MPH collection, built through a partnership between LNBio/CNPEM and Phytobios/Centroflora. The methodology included the analysis of a metabolomic database generated using the NP³ MS Workflow, containing relative quantification data and chemical structure annotations of metabolites. In addition to automated dereplication, the workflow employed molecular networking and multivariate analyses such as Multiple Correspondence Analysis (MCA) and Principal Component Analysis (PCA), which were performed in collaboration with PECEGE. A total of**11,815 protonated compounds [M+H$^+$]**were detected, of which**approximately 60% were nonredundant**(present exclusively in a single extract) and**around 67% lacked annotation**in the GNPS and/or UNPD databases, highlighting the high degree of chemical novelty within the collection. The analysis also enabled the characterization of**71 distinct chemical superclasses**, consolidated into**10 grouped superclasses**, predominantly flavonoids/phenolic derivatives and terpenes/carotenoids, underscoring the remarkable metabolic diversity among the extracts. Furthermore, the**chemical space of the collection**was successfully delineated (Figure 1), allowing clear discrimination among the grouped superclasses. Significant correlations between biomes and botanical families revealed ecological patterns in metabolite distribution. Overall, the results expand chemical annotations and reinforce the potential of Brazilian biodiversity as a source of bioactive compounds for pharmaceutical discovery.



PCA of RDKit-derived molecular properties for MPH metabolites grouped by chemical superclasses.

Agradecimentos/Acknowledgments

Lnbio/CNPEM; Phytobios/Grupo Centroflora; PECEGE for data mining

In vitro cytotoxic and antitumor properties of extracts and isolated compounds from Dizygostemon riparius

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Palavras Chave:*Dizygostemon riparius,MCF-7,Natural Products,Cytotoxicity.*

Highlights

The species*D. riparius*exhibited compounds with selective cytotoxicity against MCF-7 cells, revealing antitumor potential and highlighting the importance of natural products as therapeutic sources.

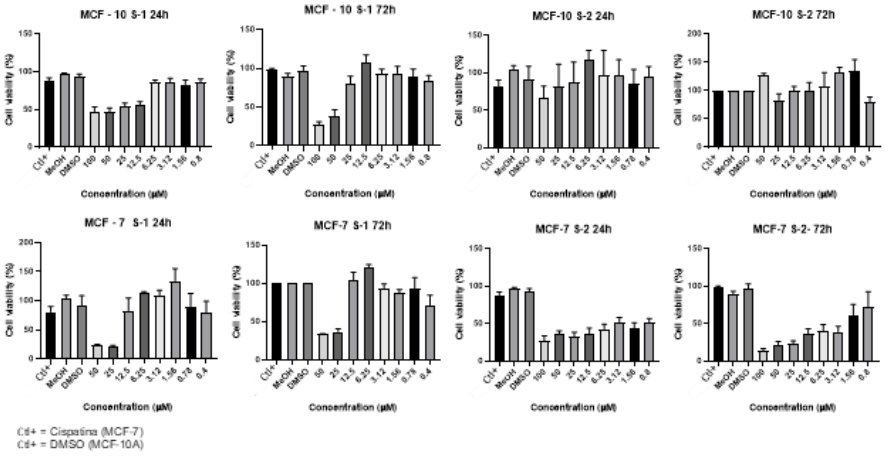
Resumo/Abstract

Cancer remains one of the major challenges of modern times, exerting a profound impact on public health (Bray et al., 2024). In this context, the search for new therapeutic alternatives includes the investigation of natural products, whose bioavailability, safety, and potential synergism with conventional drugs have attracted growing scientific interest (Izzo; Stefanska, 2025). Among these sources, plant roots stand out due to their secondary metabolites, which display wide structural diversity and diverse biological activities (Ardalani et al., 2021).

The plant species Dizygostemon riparius, collected in the municipality of São Benedito do Rio Preto, Maranhão, Brazil, is noteworthy for its still underexplored chemical and pharmacological potential. Accordingly, this study investigated the cytotoxicity of the hydroethanolic extract (S-1) and isolated compounds (S-2 and S-3), evaluating their possible antitumor activity.

In vitro cultures of the MCF-7 (breast cancer) and MCF-10A (non-tumorigenic mammary) cell lines were conducted according to Gurning et al. (2025), with adaptations. Cells were maintained in RPMI medium supplemented with 10% FBS and 1% penicillin–streptomycin, in an incubator at 37 °C, 5% CO_2, and 95% humidity. The samples were tested starting at 100 µg/mL, using serial dilutions down to 0.76 µg/mL, and cytotoxicity was assessed by the MTT assay after 24, 48, and 72 h of exposure.

In assays with MCF-7 cells, compound S-2 exhibited IC_{50} values of 25.66 µg/mL (24 h) and 3 µg/mL (48 and 72 h), while extract S-1 showed strong cytotoxic activity, with an IC_{50} of 3.8 µg/mL (24 h). Compound S-3 presented an IC_{50} of 13.25 µg/mL (24 h). All three samples showed favorable selectivity toward normal MCF-10A cells, with IC_{50} values of 7.25, 17.29, and 7.71 µg/mL, respectively.



Teste de viabilidade celular MTT em linhagens MCF7 e MCF10 após tratamento com as amostras .

Agradecimentos/Acknowledgments

I thank the PPGQ–IFMA, FAPEMA for the award of the master's scholarship, and the funding agencies CAPES, FAPESP, and CNPq.

Isolamento, Caracterização e Atividade Biológica relacionadas de Diterpenos de Plectranthus Grandis

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Palavras Chave:*Cromatografia,Terpenos,Antimicrobianas*

Highlights

Diterpenes were isolated from*Plectranthus grandis*stems by chromatography and identified by NMR, showing the species as a source of compounds with antimicrobial activity reported.

Resumo/Abstract

A espécie*Plectranthus grandis*apresenta diversos terpenos descritos na literatura, tais como barbatusina, ciclobarbatusina, entre outros compostos. Estudos recentes indicam que espécies pertencentes ao gênero Plectranthus possuem composição química diversificada, fortemente associada a diferentes atividades biológicas, destacando-se os diterpenos como a principal classe de metabólitos secundários responsáveis por propriedades terapêuticas relevantes (Porras*et al*., 2021). Entre as atividades relatadas para o gênero, podem ser mencionadas ações antimicrobiana, anti-inflamatória, gastroprotetora e antitumoral, evidenciando seu potencial farmacológico (Gáborová*et al*., 2021; Filipe*et al*., 2024).

Neste contexto, o presente trabalho descreve o isolamento de diterpenos a partir dos talos de*Plectranthus grandis*. O material vegetal foi submetido à secagem, trituração e extração por solventes orgânicos em metanol. Em seguida, realizou-se o fracionamento por cromatografia em coluna de sílica gel, possibilitando a obtenção de seis frações de polaridades crescentes. O estudo relata o isolamento e a caracterização de três terpenos obtidos das frações hexânicas, hexânica/diclorometano (50%) e diclorometano (100%).

A identificação estrutural dos compostos foi realizada por espectroscopia de Ressonância Magnética Nuclear de ^{1}H e ^{13}C, cujos dados apresentaram concordância com aqueles descritos na literatura, indicando tratar-se de 12-O-acetilferruginol, ferruginol e 6-hidroxiferruginol. Adicionalmente, foi realizado um levantamento das atividades biológicas descritas para o gênero*Plectranthus*nos últimos dez anos, reforçando a relevância desse gênero como fonte promissora de compostos naturais bioativos frente à crescente resistência microbiana (Ntungwe*et al*., 2021; Mendonça*et al*., 2023.)

Isolamento e elucidação estrutural de flavonoides das folhas de Campomanesia phaea (Myrtaceae)

Gabriela Dinis Leonardo (PG)*[1], Milena França Longue (PG)[1], Aislan Cristina Rheder Fagundes Pascoal (PQ)[1], Lucas Silva Abreu (PQ)[1].

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Palavras Chave:*Produtos Naturais,Cromatografia,Espectrometria de Massas,Ressonância Magnética Nuclear (RMN).*

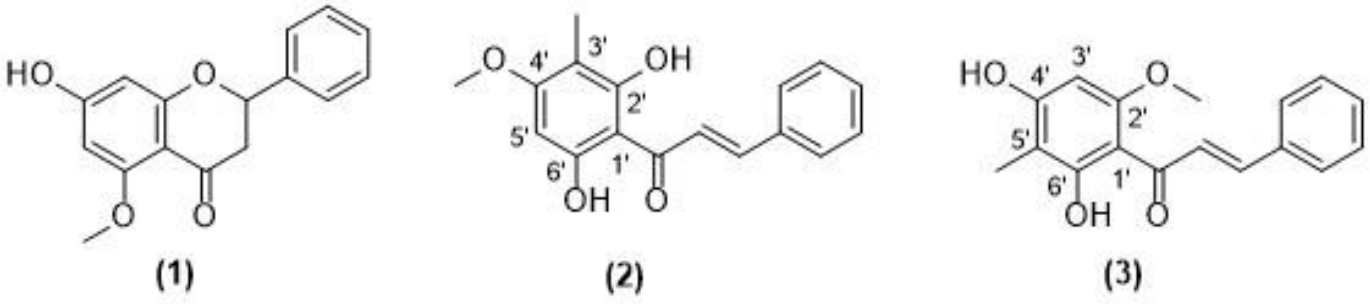
Resumo/Abstract

Campomanesia phaea(Myrtaceae) é uma espécie endêmica do Brasil, destacada pelo uso alimentício e presença de compostos bioativos[1]. Estudos preliminares do grupo de pesquisa demostraram o potencial citotóxico do extrato diclorometano das folhas dessa espécie frente as células HeLa e MG-63, porém carece de estudos sobre sua composição química. Assim, o trabalho teve como objetivo analisar o perfil por CLAE-EM e o isolamento das substâncias presentes nas folhas de*C. phaea*. O extrato foi inicialmente analisado por CLAE-EM e observou-se a presença de dois compostos majoritários que puderam ser anotados como Alpinetina**(1)**e Estercuresina**(3)**. Para confirmação dos dados observados, o extrato foi fracionado por cromatografia líquida a vácuo, seguido de purificação por cromatografia em coluna aberta. A partir das análises de RMN de ^{1}H e ^{13}C confirmou-se o isolamento da Alpinetina e da 2′,6′-dihidroxi-4′-metoxi-3′-metilchalcona[2]**(2)**, um isômero da Estercuresina (Figura 1). A diferenciação entre os isômeros é evidenciada pelos dados de RMN de ^{13}C a partir dos deslocamentos dos carbonos emδC 8,1 (3'- CH_3),δC62,4 (4'- OCH_3),δC 161,5 (C-2′) eδC 99.8 (C-5′) que diferem dos deslocamentos referentes aos carbonos correspondentes na estrutura da Estercuresina[3], evidenciando se tratarem de isômeros de posição. Esses dados mostram uma limitação da análise da espectrometria de massas em anotar isômeros de flavonoides com diferenças no anel A, evidenciando a necessidade de análises por espectroscopia de RMN. Logo, este estudo possibilitou a análise do perfil químico por CLAE–EM do extrato de diclorometano, além do isolamento e caracterização de flavonoides por RMN de ^{1}H e ^{13}C das folhas de*C. phaea,*contribuindo para o perfil químico da espécie e o desenvolvimento da Química de Produtos Naturais.

[1]RONCHI, Helena Souza*et al*.**Journal Of Education Science And Health,**2025.

[2]ZAKI, Mohamed A*et al*.**Journal Of Natural Products**, 2016.

[3]GUERRERO-PERILLA, Andrés Camilo. Tese; USP, 2021.



Estruturas químicas das substâncias isoladas das folhas de C. phaea e estercuresina

Agradecimentos/Acknowledgments

FAPERJ, CNPQ, PPGQ, CAPES, LQPN, LabNAT e LaReMN

Isolamento e identificação de um novo alcaloide aporfínico de Piper truncatum Vell.

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Palavras Chave:*Trypanosoma cruzi,atividade antiparasitária,aristolactamas*

Highlights

Quatro alcaloides incluindo um inedito na literatura, foram isolados do extrato metanolico dos galhos de*Piper truncatum*, exibindo atividade anti-*Trypanosoma cruzi*.

Resumo/Abstract

O presente trabalho tem como objetivo reconhecer compostos com ação anti-*Trypanossoma cruzi*minoritários de*Piper truncatum*. Inicialmente, os galhos foram extraídos sucessivamente com hexano e com MeOH. Uma vez que o extrato MeOH demonstrou atividade frente as formas tripomastigotas do parasita (100% de morte a 300 µg/mL) este foi submetido a partição com hexano, CH_2Cl_2 e EtOAc. Após avaliação, a fase em CH_2Cl_2 se mostrou mais ativa. A desreplicação por RMN de ^1H permitiu o reconhecimento de neolignanas dibenzilbutirolactonas previamente isoladas da espécie além de aristolactamas, sendo essas, minoritárias. Visando o isolamento de tais compostos, a fase em CH_2Cl_2 foi submetida a fracionamento em gel de sílica, fornecendo aristolactama BII (**1**), piperolactama A (**2**) e aristolactama AII (**3**) além de outro derivado (**4**). O espectro de UV de**4**mostrou absorções em l_{max} 450, 313, 300 e 234 nm, sugerindo a ocorrência de alcaloides 4,5-dioxoaporfínicos. O espectro de RMN ^1H de**4**mostrou sinais de cinco hidrogênios aromáticos em d 9,01 (m, H-11), 7,91 (m, H-8), 7,67 (m, H-9 e H-10) e 7,54 (s, H-7). Além desses, foram observados sinais atribuídos a hidrogênios de grupos metilenodioxílico em d 6,47 (s) e metílico em d 3,87 (s) além de um hidrogênio quelatado em d 12,0 (s). Tais informações permitiram sugerir a presença de um grupo metoxílico ligado diretamente ao átomo de nitrogênio, o que foi confirmado pela correlação entre o sinal de N-OMe e H-7 no mapa de correção NOESY bem como pela comparação de dados de substâncias similares descritas na literatura. Da mesma forma, o grupo metilenodioxílico foi posicionado entre C-1 e C-2 e consequentemente o grupo hidroxílico adicional foi posicionado em C-3. Finalmente, o espectro de massas de**4**mostrou sinais em*m/z*338 $[M + H]^+$ e 675 $[2M + H]^+$, em concordância com a fórmula molecular $C_{18}H_{11}O_6N$. Assim, a estrutura do composto**4**foi elucidada como*N*-metoxi-1,2-metilenodioxi-3-hidroxi-4,5-dioxo-6a,7-deidroaporfina, inédito na literatura.

Agradecimentos/Acknowledgments

CAPES,FAPESP,CNPq,UNIFESP, INSTITUTO BUTANTAN E UFABC

Isolation of a New Cytotoxic Polyketide from Talaromyces pinophilus J6 Guided by an Integrated OSMAC–Dereplication Approach

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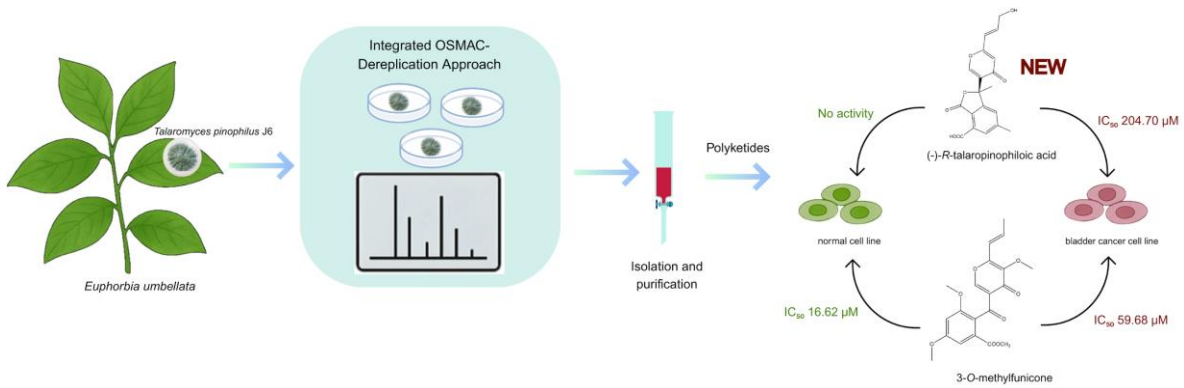
Palavras Chave:*(−)-R-Talaropinophiloic Acid,Endophytic fungus,Euphorbia umbellata,OSMAC,Dereplication*

Highlights

An integrated OSMAC-dereplication strategy revealed a distinct metabolomic profile for*Talaromyces pinophilus*J6. Two polyketides were isolated, including the new**(-)-R-talaropinophiloic acid**

Resumo/Abstract

*Euphorbia umbellata*has been used in Brazilian folk medicine for the treatment of inflammatory diseases and cancer. Its biological activities are attributed to specialized metabolites, including terpenes and phenolic compounds. Despite its well-documented pharmacological potential, the endophytic microbiota of*E. umbellata*remains poorly explored. In this study, eleven endophytic fungi (coded as J1-J11) were isolated from the aerial parts of*E. umbellata*and cultivated for 10 days at 28°C on potato dextrose agar (PDA) or PDA supplemented with different salts. Principal Component Analysis (PCA) of the crude extracts revealed that*Talaromyces pinophilus*J6 grown on PDA + $(NH_4)_2SO_4$ exhibited a distinct chemical profile. To investigate its metabolic potential, we applied an integrated strategy combining the OSMAC approach with a dereplication workflow based on an in-house high-resolution mass spectrometry (HRMS) database of*Talaromyces*metabolites. Chromatographic fractionation of the ethyl acetate extract from*T. pinophilus*J6 cultivated on PDA + $(NH_4)_2SO_4$ led to the isolation of two polyketides: the known 3-*O*-methylfunicone (**1**) and the**new (−)-R-talaropinophiloic acid**(**2**). Their chemical structures were determined by Nuclear Magnetic Resonance (NMR), Circular Dichroism (CD), and HRMS analyses. The cytotoxic activities of both polyketides were evaluated against the muscle-invasive bladder cancer cell line T24, yielding IC_{50} values of 59.68 µM for**1**and 204.7 µM for**2**, compared with 6.4 µM for the positive control cisplatin. In contrast, assays using the normal RPE-1 cell line showed that**1**displayed IC_{50} of 16.62 µM, whereas**2**was non-toxic. The lack of activity toward normal cells, combined with its cytotoxic effect on T24 cells, highlights compound**2**as highly**selective for cancer cells**. Overall, this study expands the chemical diversity known for the genus*Talaromyces*and shows endophytic fungi from*Euphorbia*species as key sources of new and bioactive polyketides.



OSMAC-dereplication guided isolation of polyketides from T. pinophilus and cytotoxic evaluation

Agradecimentos/Acknowledgments

I would like to thank the Laboratory of Microorganism Chemistry (LQM) at UFBA, CNPq for the scholarship, the Institute of Chemistry at UFBA, and all the researchers who made this work possible

Isolation of the biflavonoid agathisflavone from the leaves methanolic extract of Anacardium occidentale

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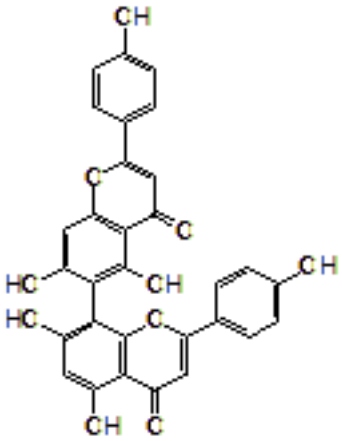
Palavras Chave:*Agathisflavone, Anacardiaceae, CLAE, RMN.*

Highlights

This study presents a phytochemical investigation focused on the isolation of the biflavonoid agathisflavone from the leaves methanolic extract of*Anacardium occidentale*.

Resumo/Abstract

Anacardium occidentale Linn., popularly known as the cashew tree, is a species native to Brazil[1] with medicinal properties, used in the treatment of inflammation, diabetes, and candidiasis[2], in addition to containing specialized metabolites associated with various biological activities[3]. Among the flavonoids identified, agathisflavone stands out, to which hepatoprotective and antioxidant activities have been attributed[4].The objective of this work was to isolate the biflavonoid agathisflavone from the leaves of*A. occidentale*, using flash column chromatography, and Sephadex LH-20 chromatography, as well as to analyze the isolated compound by High-Performance Liquid Chromatography (HPLC). Initially, the methanolic extract of the leaves was subjected to liquid-liquid partitioning, obtaining fraction A. Oc-5B (EtOAc). This fraction was then subjected to a vacuum liquid chromatography (VLC) on silica gel ($CHCl_3$, $CHCl_3$:MeOH 95:5; 9:1; 8:2 (v/v), and MeOH), resulting in fraction A. Oc-8C (9:1 v/v), which underwent an additional purification step by size-exclusion chromatography using MeOH, resulting in fraction A. Oc-13O (124 mg). The isolated compound showed a yield of 0.038 % relatiove to dry leaves, a value higher than that described in the literature (0.015%)[5]. Finally, the fraction was analyzed by HPLC, which indicated the isolation of the compound of interest with a purity of 99 %. Preliminary structural determination of the isolated compound was performed by ^1H NMR analysis. In this context, the results obtained corroborate previously reported data, reinforcing the feasibility of isolating agathisflavone from*A. occidentale*.



Chemical structure of agathisflaovna

Agradecimentos/Acknowledgments

This research was supported by CAPES, CNPq and FAPESP.

LC–MS-Based Dereplication of Metabolites from Stems and Leaves of the Parasitic Plant Psittacanthus cordatus

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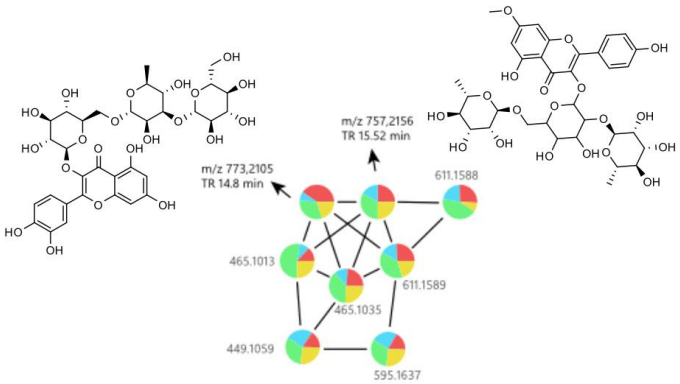
Palavras Chave:*natural products, plant parasitism, phytochemistry, mass spectrometry, secondary metabolism.,natural products,plant parasitism,phytochemistry,mass spectrometry,secondary metabolism*

Highlights

Untargeted metabolomics uncovered chemical profile of leaves and stems from a parasitic plant. Presence of O-glycosited flavonoid, quercetins, flavones and hidrolyzed tanins.

Resumo/Abstract

*Psittacanthus cordatus*is a parasitic plant from the Loranthaceae family that obtains water and nutrients from its hosts through haustoria, specialized structures connected to the host vascular system. While they can invade natural habitats and agricultural crops, reducing productivity and causing financial loss, their unique parasitic biology may also provide biomolecules of pharmaceutical interest. Nevertheless, research on parasitic plants' chemical profile is limited, restricting our understanding of their biological and therapeutic potential, emphasizing the need for descriptive phytochemical studies to elucidate the chemical diversity and biological potential. In this study, the phytochemical profile of*P. cordatus*leaves and stems collected from four distinct host species were investigated using a dereplication approach, employing untargeted metabolomics with HPLC-ESI-qTOF-MS and GNPS libraries. As a result, chemical profiling revealed that, in the leaves, the majority of the annotated compounds corresponded to O-glycosylated flavonoids, flavonols and quercetins, like quercetin-3-O-glc-1-3-rham-1-6-glucoside and nicotflorin, whereas triterpenoids, tryptophan-derived alkaloids and hydrolysable tannins, like 3,3'-Di-O-methylellagic acid, were predominantly detected in the stems. Those found compounds are commonly associated with plant defense and adaptation mechanisms, as observed in protection against oxidative stress, UV radiation, and biotic stressors such as allelopathic, herbivores and pathogens, but also shows molecules with pharmaceutical interest, as antioxidant effect and anti-inflammatory. The dereplication methodology facilitates the identification of previously isolated compounds using NP databases and the metabolomic approach contributed to a better understanding of parasite chemical profile, but alsoreinforces the pharmaceutical potential of*P. cordatus*, encouraging further biological assays of its extracts as a next stage of this study.



MS/MS molecular networking of Psittacanthus cordatus flavonoid glycosides and proposed structures

Agradecimentos/Acknowledgments

The authors acknowledge the School of Pharmaceutical Sciences FCF-USP for providing the infrastructure and FAPESP (processes 2024/18203-0; 2022/08191-9) for financial support.

LC–MS/MS-Based Dereplication of Discriminant Metabolites in Psittacanthus acinarius Growing on Distinct Host Species.

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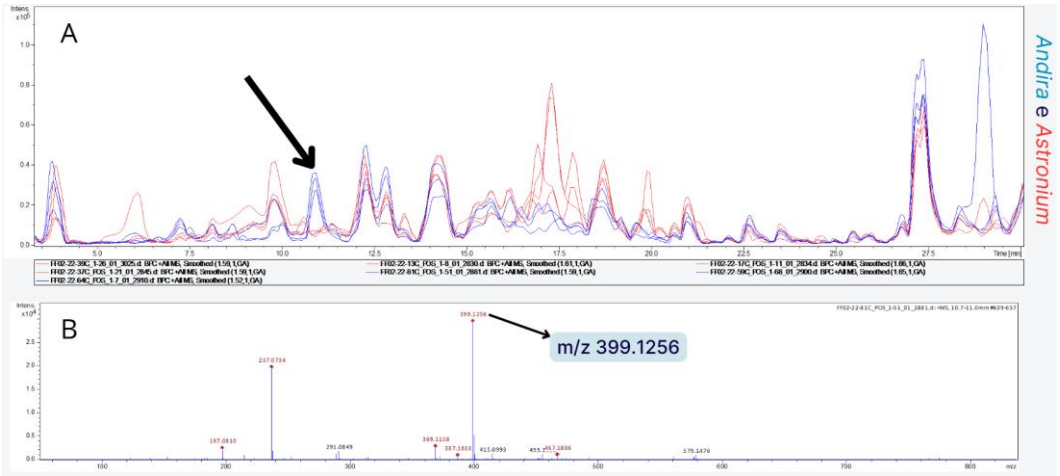
Palavras Chave:*Metabolomics,Natural Products,Parasite plants,Phytochemical profile,Isolation*

Highlights

Metabolomic analyses allow the evaluation of substance interactions in parasitic relationships, revealing isolated compounds with pharmacological potential.

Resumo/Abstract

Parasitic plants rely on a specialized organ, the haustorium, which invades the host vascular system and enables the exchange of water and nutrients, influencing chemical composition. This study applied an untargeted LC–MS/MS-based metabolomic and dereplication approach to investigate host-dependent metabolic modulation in the hemiparasitic plant*Psittacanthus acinarius*associated with*Andira inermis*and*Astronium fraxinifolium*. Leaves and stems from parasites, parasitized hosts, and non-parasitized hosts were extracted using methanol and sequential maceration with hexane, ethyl acetate, and ethanol. Chemical profiling was performed by UPLC–qTOF-MS in positive ionization mode, with data processing in DataAnalysis and MZmine, molecular networking in GNPS, and multivariate analyses in MetaboAnalyst. As no significant chemical differences were observed among hosts, comparisons focused on parasites associated with each species. Distinct host-dependent metabolic signatures were detected in*P. acinarius*. A discriminant ion at m/z 399.1252 (RT 10.8 min), tentatively identified as loganic acid (mussaenosidic acid), was exclusively found in parasites growing on*A. inermis*and in the corresponding parasitized host, while absent in non-parasitized samples. In contrast, parasites associated with*A. fraxinifolium*exhibited flavonoid-related features, including quercetin (m/z 303.0497). Multivariate analyses confirmed clear discrimination between parasite groups, with m/z 399.1252 emerging as a key marker. This compound was isolated by chromatographic techniques and submitted to NMR analyses for structural confirmation. These findings highlight host-driven chemical modulation in*P. acinarius*and demonstrate the value of untargeted metabolomics in parasite–host interaction studies.



BPC shows a 10.5–11.0 min peak exclusive to parasites on A. inermis (A), with ion m/z 399.1256 (B).

Agradecimentos/Acknowledgments

The authors acknowledge the financial support from FAPESP (grant no. 2024/15443-0 and 2022/08191-9) and the Laboratory of Pharmacognosy for technical support.

Mapping phytochemical profiles of arboreal plants from Amazonian agroforestry systems

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Palavras Chave:*Agroforests systems; Mass profiling; Amazonian biodiversity*

Highlights

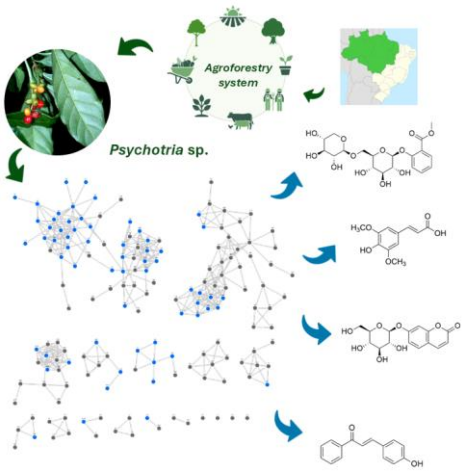
Chemical mapping supports sustainable valorization of Amazonian biodiversity.

Resumo/Abstract

Amazonian plant biodiversity is a promising source of secondary metabolites with enormous biological and chemical potential [1]. For the past decades, agroforestry systems have been sought by the Amazonian people as an effective strategy to combine agricultural output with environmental preservation [2]. In this study, arboreal species belonging to several agroforestry systems present in the metropolitan region of Manaus were investigated. These species include*Solanum paniculatum*(leaves and flowers),*Swartzia corrugata*,*Garcinia acuminata*,*Muriri ulei*,*Handroanthus barbatus*,*Quiina rhytidopus*,*Handroanthus serratifolius*,*Paramachaerium ormosioides*,*Pseudobombax munguba*(leaves and trunk),*Picrasma crenata*(trunk) and*Psychotria cartagenensis*(leaves). The plant material was collected in the municipality of Manacaupuru, Amazonas State, dried in an oven with air circulation at 40ºC and later milled to a fine powder. Ten grams of each sample were extracted using 50 mL of boiling water to target medium- and high-polarity metabolites, and the resulting extracts were subsequently loaded onto an SPE cartridge for cleanup and concentration. The extracts were analyzed by liquid chromatography coupled to high-resolution mass spectrometry (LC-MS/MS), using dereplication strategies for the identification and annotation of the compounds present using the GNPS (https://gnps.ucsd.edu/)database. Dereplication data pointed to phenylpropanoids, coumarins and chalcones as the main classes of the annotated compounds (Figure 1). This study aims to contribute to the chemical mapping of agroforestry systems, expanding the knowledge about their metabolic diversity and providing support for future chemical and biological investigations, thus promoting the sustainable valorization of Amazonian biodiversity.

[1] Conrado*et al*.*Revista Brasileira de Farmacognosia*, 2024.

[2] Pauletto*et al*.*Land*, 2025.



Annotated compounds from agroforestry systems using dereplication tools

Agradecimentos/Acknowledgments

CNPq; FAPEAM; INPA; UEA

Meleagrin from Penicillium chrysogenum: antibacterial activity and FabI-targeted in silico insights against antimicrobial resistance

Simone dos Santos Grecco (PQ)*[1], Jackson Monteiro (PQ)[1], Gabriel Martins da Silva (PG)[2], Marisi Gomes Soares (PQ)[3], Renata Pascon (PQ)[1], Marcelo Afonso Vallim (PQ)[1], Rodrigo Cayô da Silva (PQ)[1], Daniela G. G. Rando (PQ)[1], Patricia Sartorelli (PQ)[1].

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Palavras Chave:*Endophytic fungi,Penicillium chrysogenum,meleagrin,antibacterial activity,FabI inhibition*

Highlights

Integrated*in vitro*and*in silico*analysis identify meleagrin as a selective antibacterial agent with plausible FabI-mediated activity.

Resumo/Abstract

The rapid emergence of antimicrobial-resistant pathogens has intensified the search for new antibacterial agents from natural sources. Endophytic fungi associated with medicinal plants are recognized as prolific producers of structurally diverse secondary metabolites with relevant biological activities. In this study, meleagrin, isolated from the endophytic fungus*P. chrysogenum*obtained from*Duguetia lanceolata*, was evaluated for its antibacterial potential through*in vitro*and*in silico*approaches. Antibacterial activity was assessed against*Staphylococcus aureus*(ATCC 29213) and*Escherichia coli*(ATCC 25922), as well as multidrug-resistant isolates: methicillin-resistant*S. aureus*(MRSA, SCCmec II) and carbapenem-resistant*Enterobacter cloacae*(ECL79101, producing KPC, NDM or IMP). Meleagrin showed selective activity against susceptible strains, with MIC values of 0.002 mg.mL^{-1} for*S. aureus*and 0.004 mg.mL^{-1} for*E. coli*, while no significant activity was observed against the resistant isolates, suggesting a target-mediated mechanism rather than nonspecific toxicity. Positive controls showed MIC values of 0.006 mg.mL^{-1} for triclosan (against*S. aureus*,*E. coli*and MRSA) and >0.032 mg.mL^{-1} for chloramphenicol (against the*E. cloacae*clinical isolate).*In silico*analyses indicated favorable pharmacokinetic properties. Molecular docking against enoyl-acyl carrier protein reductase (FabI), an essential enzyme in bacterial fatty-acid biosynthesis, showed favorable binding to FabI from*S. aureus*(4ALI) and*E. coli*(1C14), with energies ofΔG−6.76 and −6.91 kcal.mol^{-1}, comparable to triclosan (ΔG−7.22 and −7.14 kcal.mol^{-1}). Similar binding across FabI orthologs supports a conserved interaction within the catalytic pocket, reinforcing FabI inhibition as a plausible mechanism. Meleagrin emerges as a promising antibacterial metabolite from an endophytic fungal source, warranting further investigation as a natural-product lead against antimicrobial resistance.

Agradecimentos/Acknowledgments

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of São Paulo, São Paulo Research Foundation (FAPESP), CAPES and CNPq.

Metabolomic and chemometric analysis of leaf extracts from seven Banisteriopsis species by UPLC-MS/MS and evaluation of their biological potential.

Grazielle Jesus dos Santos (PG)*[1], Jaqueline Munise Guimarães da Silva (PG)[1], Maria Fernanda Alvani (PG)[1], Isabely Amadeu Montanha (PG)[1], Rafael Felipe de Almeida (PQ)[2], Maria Carolina Carneiro (PG)[1], Nilton Syogo Arakawa (PG)[1], Ana Carolina Jacob Rodrigues (PG)[1], Wander Rogério Pavanelli (PQ)[1], Maria Luiza Zeraik (PQ)[1].

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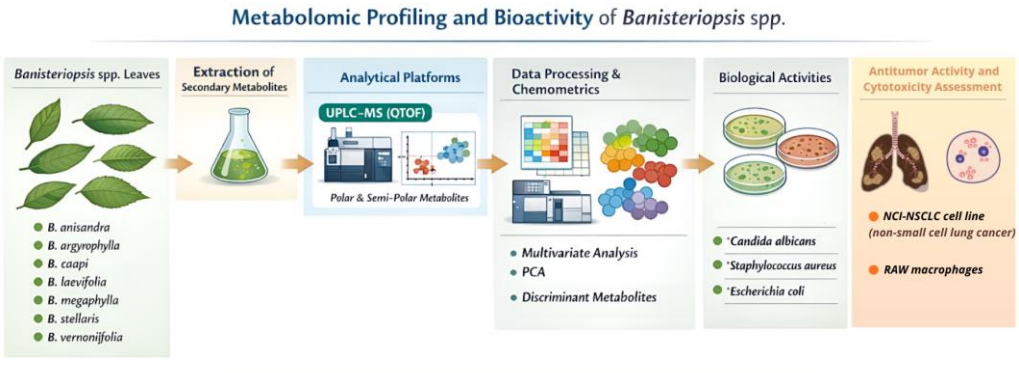
Palavras Chave:*Secondary metabolites,PLS-DA,Antifungal,Antibacterial,Antitumor*

Highlights

First report on the integration of metabolomic profiling, interspecific multivariate analysis, and bioactive potential of seven Banisteriopsis species.

Resumo/Abstract

The genus Banisteriopsis has attracted increasing scientific interest due to the remarkable diversity of secondary metabolites produced by its species, as well as their ecological and pharmacological relevance. However, studies integrating metabolomics and chemometrics remain scarce. In this study, an untargeted metabolomic analysis was performed on leaf extracts from seven Banisteriopsis species (B. anisandra, B. argyrophylla, B. caapi, B. laevifolia, B. megaphylla, B. stellaris, and B. vernoniifolia) using ultra high performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS). The metabolomic profiles revealed a high abundance of alkaloids, flavonoids, and phenolic compounds, evidencing pronounced interspecific metabolic diversity. Chemometric analyses enabled the identification of discriminant metabolites among the species. Multivariate partial least squares discriminant analysis (PLS-DA) identified 15 compounds, including luteolin that discriminate among the seven Banisteriopsis species. These compounds accounted for the clear metabolomic differentiation among the evaluated species, representing the first integrated metabolomics based approach applied to the interspecific discrimination of Banisteriopsis leaves. In parallel, the biological activities of the extracts were evaluated. Antifungal and antibacterial assays were conducted against C. albicans ATCC 10231, Staphylococcus aureus ATCC 25925, and E. coli ATCC 25922. Extracts active against C. albicans exhibited fungicidal effects at 2000 µg mL^{-1}, whereas those active against bacterial strains showed bacteriostatic behavior. In addition, antitumor activity is currently being assessed using the NCI-NSCLC cell line, along with cytotoxicity assessment in J774A.1 macrophages. Overall, these findings highlight the high biotechnological potential of the genus and reinforce natural product bioprospecting as a promising strategy for the discovery of new therapeutic agents.



Integrative metabolomic and biological workflow of Banisteriopsis leaves (Malpighiaceae).

Agradecimentos/Acknowledgments

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Metabolomic study of seeds from different Crotalaria species and evaluation of their herbicidal activity

CRISTIANE ISAAC CERCEAU (TC)*[1], TAINÁ SILVA FIGUEIREDO (PG)[1], Antonio Jacinto Demuner (PQ)[1], Elson Santiago de Alvarenga (PQ)[1], Guilherme Julião Zocolo (PQ)[2], Marcelo Henrique dos Santos (PQ)[1].

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Palavras Chave:*Metabolomics, Herbicidal Activity, Pyrrolizidine Alkaloids, Monocrotaline, Natural Products.*

Highlights

*Crotalaria*seed extracts strongly inhibit seedling root growth. Metabolomic profiles distinguish*C.juncea*from*C.spectabilis*. UPLC-QTOF-MSE and OPLS-DA enable clear discrimination.

Resumo/Abstract

Plants of the genus*Crotalaria*exhibit rapid growth and are easy to cultivate, being widely used in agriculture for the control of insects and larvae. These properties are directly associated with the production of specialized metabolites with biological activity. This study aimed to investigate the metabolomic profiles of seeds from different species of the genus*Crotalaria*, as well as to evaluate the herbicidal activity of their respective extracts. The research was motivated by the development of more efficient and sustainable agricultural protectants, within a framework that values the prospection of bioactive compounds derived from Brazilian biodiversity. Ethanolic extracts and acidic aqueous solution extracts were prepared from the seeds of*Crotalaria juncea*and*Crotalaria spectabilis*. Chemical characterization was carried out using Ultra-Performance Liquid Chromatography coupled with High-Resolution Mass Spectrometry (UPLC-QTOF-MSE), and the resulting data were subjected to multivariate statistical analyses, including the OPLS-DA model. Biological evaluation consisted of germination bioassays to determine the effects of the extracts on early growth of different plant species. Metabolomic analysis revealed distinct chemical profiles between the studied species, with a predominance of the alkaloid monocrotaline in*C.spectabilis*and globiferine in*C.juncea*. All extracts exhibited notable herbicidal activity, mainly characterized by pronounced inhibition of seedling root development. Monocrotaline, a pyrrolizidine alkaloid, showed greater inhibitory efficacy than the flavonoid quercetin, supporting the high phytotoxic potential of this class of secondary metabolites. Furthermore, no marked selectivity was observed between monocotyledonous and dicotyledonous species, suggesting a broad spectrum of action. Therefore,*Crotalaria*seed extracts represent a promising source of bioactive compounds for the development of natural herbicides with broad-spectrum activity.

Agradecimentos/Acknowledgments

We thank CNPq, FAPEMIG, and FINEP for financial support, and EMBRAPA for the analyses performed.

Molecular Networking-Guided Isolation of Flavonoids from Ziziphus by Countercurrent Chromatography (CCC)

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Palavras Chave:*Ziziphus; Countercurrent Chromatography (CCC); GNPS; Triphasic Solvent Systems; Natural Products Isolation.*

Highlights

CCC as an efficient support-free liquid-liquid partition tool for Ziziphus; Application of triphasic solvent systems (TPSS) for Ziziphus fractionation; Molecular networking-guided isolation of flavonoid

Resumo/Abstract

The genus*Ziziphus*(Rhamnaceae) stands out in the bioprospecting of secondary metabolites such as cyclopeptide alkaloids, triterpenes, and flavonoids, with inhibitory potential against α-glucosidase. This study presents Countercurrent Chromatography (CCC), a support-free liquid-liquid partition technique, as a pivotal tool for the phytochemical investigation of the native species*Z. joazeiro*and*Z. undulata*. Ethanolic and hydroalcoholic extracts from leaves and twigs were obtained (yields from 7.7% to 15.0%), followed by sequential liquid-liquid partitioning and acid-base extraction using a green chemistry protocol with ethyl acetate and chloroform to obtain alkaloid-enriched fractions (AEF). CCC was optimized for direct isolation and broad-spectrum fractionation: for*Z. joazeiro*(EBFZJ), the biphasic HEMWat (6:1:6:1,*v/v/v/v*) system enabled the single-step isolation of ZJS1, identified by ^{1}H NMR as methyl pheophorbide A (MPhA). For*Z. undulata*(EBFZU), the use of Triphasic Solvent Systems (TPSS) (Hex:AcOMe:ACN:H_2O 2:1:2:2,*v/v/v/v*) was introduced, achieving high stationary phase retention (*Sf*> 86%) and allowing the separation of constituents with a wide range of polarity in a single run. Concurrently, the dichloromethane fraction was purified by gel permeation (Sephadex LH-20), yielding glycosylated flavonoids confirmed by TLC (NP/PEG reagent), which are currently under structural elucidation by NMR and MS analyses. Molecular networking analysis (FBMN-GNPS) revealed the metabolic complexity of the species, grouping clusters that enabled the dereplication of cyclopeptides and flavonoids. The results demonstrate that CCC overcomes conventional chromatography limitations, such as irreversible adsorption, being essential for phytochemical mapping and the discovery of new therapeutic targets for diabetes management.

Agradecimentos/Acknowledgments

The authors gratefully acknowledge the financial and institutional support from CNPq, FAPERJ, UFRJ, and IPPN.

Nanoemulsions enhance antischistosomal activity of bioactive acetogenins from Porcelia macrocarpa in a preclinical model

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Palavras Chave:*Acetogenins, Porcelia macrocarpa, Drug delivery, Nanoformulation, Schistosoma mansoni,Acetogenins,Porcelia macrocarpa,Drug delivery,Nanoformulation,Schistosoma mansoni*

Highlights

A nanoemulsified oil–water drug delivery system enhanced the bioactivity of acetogenins isolated from*Porcelia macrocarpa*in an*in vivo Schistosoma mansoni* model.

Resumo/Abstract

Acetogenins isolated from*Porcelia ponderosa*previously demonstrated potent in vivo activity against*Schistosoma mansoni*. Based on these findings, two fractions enriched in chemically related acetogenins were obtained from*Porcelia macrocarpa*seeds: fraction A (compounds**1**and**2**; 93:07) and fraction B (compounds**3**and**4**; 98:02). After chemical characterization by NMR and ESI-HRMS, fractions A and B were administered as a single oral dose (400 mg/kg). Two weeks after treatment, animals were euthanized, and efficacy was assessed by determining worm burden reduction (WBR) and egg burden reduction (EBR). Fractions A and B produced WBR values of 81.9% and 92.9% and EBR values of 94.4% and 97.7%, respectively, compared with reductions of 88.2% (WBR) and 87.0% (EBR) observed for the reference drug praziquantel (PZQ). At reduced doses, fractions A and B achieved WBR values of 62.0% and 75.0% at 200 mg/kg and 60.0% and 40.7% at 100 mg/kg, whereas PZQ yielded reductions of 56.7% and 15.7% at the same doses. Compound**3**was subsequently isolated by HPLC and evaluated under identical conditions, resulting in WBR values of 53.2%, 42.4%, and 23.4% at doses of 400, 200, and 100 mg/kg, respectively. These results suggest a synergistic effect among the compounds, as the enriched fraction exhibited greater efficacy than the isolated constituent. Based on this outcome, fraction B was selected for the development of a nanoemulsified drug delivery system. Four oil–water nanoemulsion formulations (F1–F4) were prepared and characterized by rheological analysis and dynamic light scattering (particle size and zeta potential). Among them, formulation F2 showed the most favorable physicochemical properties and was selected for in vivo evaluation at the lowest dose, achieving a WBR of 79.0%. Notably, F2 not only doubled the previously observed bioactivity at this dose but also reduced egg burden by 56.7%, an effect not observed with the non-formulated fraction.

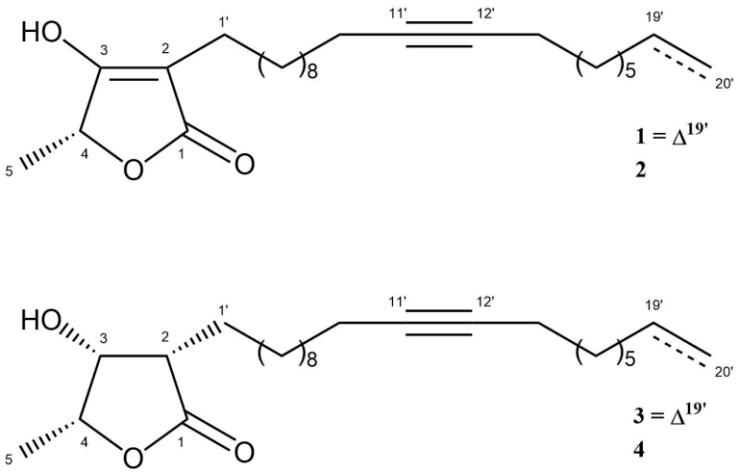


Figure 1. Chemical structures of acetogenins from fractions A (1 and 2) and B (3 and 4)

Agradecimentos/Acknowledgments

CAPES, CNPq and FAPESP

Nanoemulsões de timol: influência da matriz tensoativa na estabilidade físico-química e atividade antifúngica frente a Alternaria sp.

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Palavras Chave:*Nanoemulsões,Timol,SDBS,Fungicida*

Highlights

Thymol nanoemulsions were stabilized at HLB 13. SDBS provided electrostatic stability (-45.32 mV) for 4 months. Thymol-loaded systems enhanced antifungal activity with a 50 ppm MIC.

Resumo/Abstract

O timol é um monoterpeno fenólico amplamente investigado por sua atividade antifúngica, embora sua baixa solubilidade aquosa limite aplicações em sistemas dispersos. Este trabalho objetivou desenvolver nanoemulsões de timol e avaliar a influência do dodecilbenzenossulfonato de sódio (SDBS) na estabilidade físico-química e na atividade biológica frente ao fungo*Alternaria*sp. As formulações foram preparadas por homogeneização de alto cisalhamento, utilizando os surfactantes não iônicos Tween 80 e Span 20, na presença e ausência de SDBS como agente auxiliar de estabilidade. As propriedades foram monitoradas por tamanho médio de partícula, índice de polidispersão (PDI) e potencial zeta. O ajuste do balanço hidrofílico-lipofílico (HLB) da matriz para o valor 13 foi determinante para a estruturação do sistema. Enquanto as formulações compostas apenas por tensoativos não iônicos apresentaram instabilidade (separação de fases), a incorporação de uma pequena fração de SDBS promoveu estabilização eletrostática robusta. As nanoemulsões resultantes mantiveram-se estáveis por 4 meses, com diâmetro médio de 101,6 nm, PDI de 0,3 e potencial zeta de -45,32 mV. Nos ensaios biológicos, as matrizes de Tween 80/Span 20 foram inativas. Contudo, a matriz contendo SDBS exibiu atividade antifúngica intrínseca, inibindo totalmente o crescimento fúngico na diluição equivalente àquela que conteria 500 ppm de ativo. Em contraste, a nanoemulsão completa (timol + SDBS) demonstrou eficácia superior, com Concentração Inibitória Mínima (CIM) de 50 ppm. Os resultados evidenciam que, embora o SDBS atue como agente inibidor na matriz, sua associação com o timol potencializa a resposta biológica, reduzindo drasticamente a dose necessária para o controle de*Alternaria*sp. e destacando a importância da matriz tensoativa no design de nanocarreadores funcionais.

Agradecimentos/Acknowledgments

Agradecemos ao PPGMQ-MG, à Fapemig, à CAPES e ao CNPq pelo apoio financeiro; à UFV-CRP e ao Laboratório de Desenvolvimento de Agroquímicos Naturais pelo suporte técnico e infraestrutura para este trabalho.

Nature's Shield: Leveraging Yeast Metabolomics for Sustainable Sunscreens

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Palavras Chave:*Metabolomic, yeasts, biomolecule, biotechnology, mycosporine.*

Highlights

A metabolomic approach for biotechnological sunscreens

Resumo/Abstract

Ultraviolet Radiation (UVR) poses significant risks to human health, most notably its role in the pathogenesis of skin cancer. While organic and mineral sunscreen filters are standard in photoprotection, their persistent environmental toxicity has sparked an urgent search for sustainable alternatives. In this context, environmental yeasts have emerged as promising sources of biomolecules with photoprotective and biotechnological potential. The Microbial Interactions Laboratory at UNIFESP maintains a collection of environmental yeasts, including some mycosporine producers. This work presents preliminary chemical analysis of new yeasts with biotechnological potential, with focus on the investigation and characterization of their metabolic fingerprint. For metabolomic analysis and chemical dereplication HPLC/DAD-HRMS data were applied. MS-DIAL, MZmine, and GNPS2 were used for data processing, metabolite annotation, and molecular networking. These integrated tools enabled the study of the chemical diversity produced by understudied yeast strains, leading to the identification of unknown mycosporines. Other compounds of commercial and biotechnological interest can be also identified, reinforcing the potential of environmental yeasts as sustainable sources of new natural products.

Agradecimentos/Acknowledgments

FAPESP
CAPES
CNPQ
LABiorg

Neolignanas isoladas de Nectandra paranaensis (Lauraceae) apresentam atividades anti-S. mansoni in vivo moduladas de acordo com a estereoquímica

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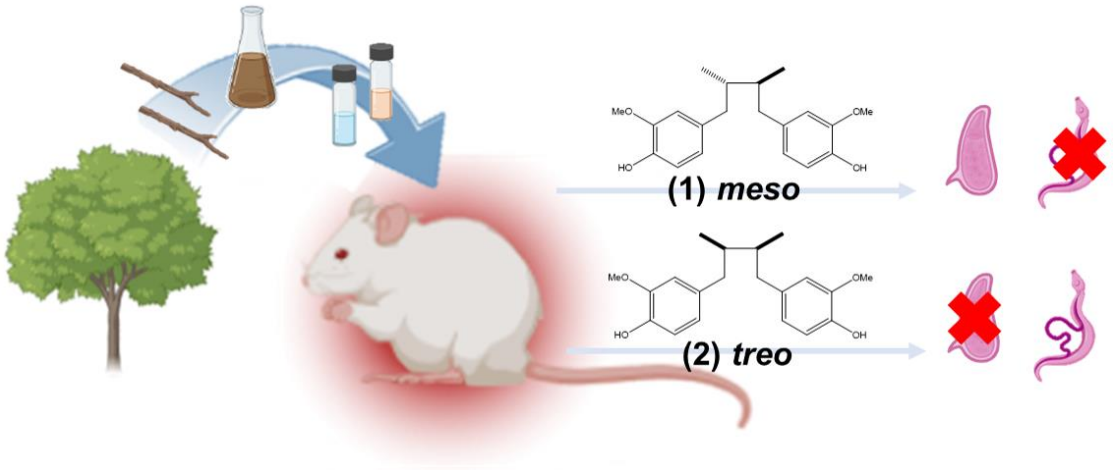
Palavras Chave:*schistosomiasis, lignan, dibenzylbutane, guaiaretic acid,esquistossomose,lignanas,dienzilbutânicas,ácido guaiarético,diastereosiômeros*

Highlights

Complementary biological profiles highlight diastereomeric neolignans from*N. paranaensis*as promising models for anti-*S. mansoni*prototypes discovery.

Resumo/Abstract

A química de produtos naturais é reconhecida por sua forte contribuição na busca de protótipos bioativos e, a fim de contribuir com a prospecção de novos compostos antiparasitários, a espécie*Nectandra paranaensis*(Lauraceae), de fitoquímica inédita, tem sido estudada. O extrato hexânico obtido dos galhos apresentou atividade*in vitro*contra*S. mansoni*, parasita causador da esquistossomose, promovendo 100% de mortalidade dos vermes após 24h (200 µg/mL) e 48h (50 µg/mL). Seguindo uma abordagem de fracionamento biomonitorado, foram obtidas duas, dentre 28 frações, que mantiveram a atividade anti-*S. mansoni*observada para o extrato bruto. A desreplicação destas frações por RMN de ^{1}H e ^{13}C sugeriu a presença de neolignanas dibenzilbuânicas, classe previamente associada à atividade esquistossomicida. O avanço do fracionamento cromatográfico levou ao isolamento e caraterização estrutural (RMN de ^{1}H e ^{13}C, e EM) dos ácidos*meso-(R,S)*-(**1**) e*treo-(R,R)*-diidroguaiarético (**2**), inéditos em*Nectandra,*cujas configurações absolutas foram determinadas por dicroísmo circular eletrônico. Em ensaios*in vivo*,**1**e**2**foram administrados a camundongos infectados a 400 mg/kg. Após duas semanas do tratamento, enquanto o composto**1**havia reduzido 53% da carga de vermes,**2**não promoveu efeito significativo, e o controle positivo praziquantel promoveu 88% de redução. Por outro lado,**2**reduziu em 100% o número de ovos nas fezes e em 70% a carga de ovos imaturos no intestino, similar ao controle praziquantel (100% e 87% de redução, respectivamente), enquanto**1**não provocou efeito. Tanto a eliminação dos vermes como a redução da ovoposição são essenciais na busca de compostos esquistossomicidas. Portanto, os perfis de atividade de**1**e**2**sugerem efeito complementar e evidenciam o papel central da estereoquímica na modulação da resposta biológica, destacando esses compostos como modelos de interesse para investigações futuras acerca de alvos moleculares, incluindo o uso de ferramentas*in silico*.



Os diastereosiômeros 1 e 2 apresentam atividades complementares em modelo in vivo de S. mansoni.

Agradecimentos/Acknowledgments

FAPESP, CNPq, CAPES.

UFABC, UNG.

Networking analysis for the dereplication of polar substances in extracts from parasitic and host species.

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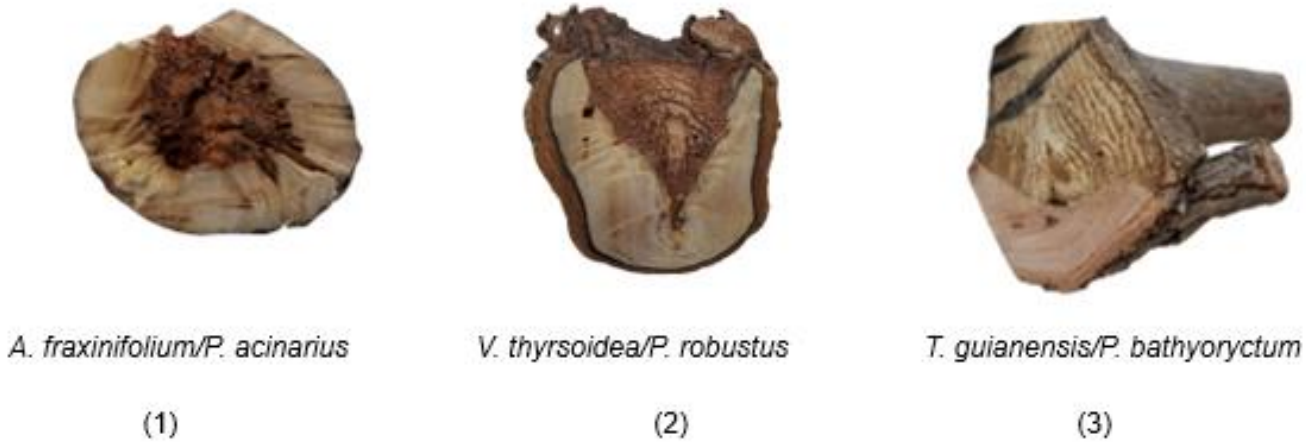
Palavras Chave:*Natural products,Phytochemistry,Secondary metabolites,Parasitic plant*

Highlights

HPLC and LC-MS/MS analysis of the parasite–host insertion point reveals similar chemical profiles, suggesting metabolite sharing between tissues.

Resumo/Abstract

The haustorium promotes the direct connection between vascular systems in plant parasitism, mediating the transfer of water, nutrients, and metabolites between parasite and host. To investigate the chemical profile of the host–parasite interface, haustoria from*Astronium fraxinifolium/Psittacanthus acinarius*,*Vochysia thyrsoidea/Psittacanthus robustus*, and*Tapirira guianensis/Phoradendron bathyoryctum*were collected in the Pantanal (February 2024). After separation of parasite and host tissues, the plant material was subjected to sequential extraction with hexane, ethyl acetate, and ethanol, and the extracts were analyzed by LC-MS/MS (Q-TOF). In the*A. fraxinifolium/P. acinarius*system, few coincident ions were observed between tissues; m/z 543.3275 and 485.3241 (RT 22 min) occurred exclusively in the host, although they were also detected in*V. thyrsoidea*and in the ethanolic extract of*P. robustus*. For*V. thyrsoidea/P. robustus*, the shared ion m/z 437.1936 (RT 24.2 min) was identified. In*T. guianensis/P. bathyoryctum*, the ions m/z 377.0832 and 303.0494 (compatible with quercetin) were common to both tissues, in addition to m/z 437.1927, 419.2755, and 425.2141. Among metabolites previously described in parasitic plants, only quercetin has been reported as a possible haustorium-inducing factor. The other detected substances do not present functional annotations associated with the formation of this structure, despite the correspondence of some molecular formulas with classes of terpenoids. Taken together, the data indicate that the chemical profile of the mature haustorium remains poorly characterized, highlighting the need for further studies to better understand its role in the physiological and metabolic interaction between parasites and hosts.



Haustorial systems 1, 2, and 3, respectively, corresponding to the studied parasite–host systems.

Agradecimentos/Acknowledgments

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Obtaining Tenebrio molitor Proteins for Application as a Functional Ingredient in Sustainable Cosmetics.

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Palavras Chave:*Tenebrio molitor,protreins,cosmetics,antioxidant*

Highlights

Formulation of natural cosmetic products using protein from the mealworm insect*Tenebrio molitor.*

Resumo/Abstract

The cosmetic industry has been seeking sustainable alternatives to replace synthetic ingredients with raw materials of low environmental impact and high functional value, with a focus on the use of natural ingredients in cosmetic dermatology (Baumann, Woolery-Lloyd & Friedman, 2009). In this context, insect proteins, especially from Tenebrio molitor, have stood out as an innovative source due to their high protein content, bioactivity, and favorable amino acid profile. The aim of the work was to develop and apply protocols for the extraction and evaluation of proteins, as well as the formulation and application of sustainable cosmetics. The protein extraction was carried out by agitation in an alkaline medium (pH 10.0), followed by centrifugation, adjustment of the pH to the isoelectric point (pH 4.5), purification by dialysis, and subsequent lyophilization. The quantification of proteins was conducted using the Bradford method (Bradford, 1976). The obtained protein material was characterized for the presence of functional groups by Fourier-transform infrared spectroscopy (FTIR), in addition to the evaluation of techno-functional properties such as solubility and morphology (SEM). Based on evidence from the literature on the inhibition of the tyrosinase enzyme in skin whitening processes (Maeda & Fukuda, 1991) and the high antioxidant activity associated with the bioactive potential, it was evaluated thru antioxidant assays (DPPH and ABTS) and in vitro cytotoxicity tests. As a product, we developed prototypes of creams and lotions containing the extracted protein material, formulated based on protocols described in the literature, which were subjected to physicochemical stability tests, in accordance with studies demonstrating the feasibility of using Tenebrio molitor derivatives in cosmetics (Verheyen et al., 2023). The results indicated the potential of T. molitor as a safe and promising functional ingredient for sustainable cosmetic applications.

Agradecimentos/Acknowledgments

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Optimization of 3-O-methylfuniconone biosynthesis by Talaromyces pinophilus J6 and its inhibitory activity against Helicobacter pylori.

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Palavras Chave:*Endophytic fungi,antimicrobial,OSMAC,specialized metabolites,polyketide.*

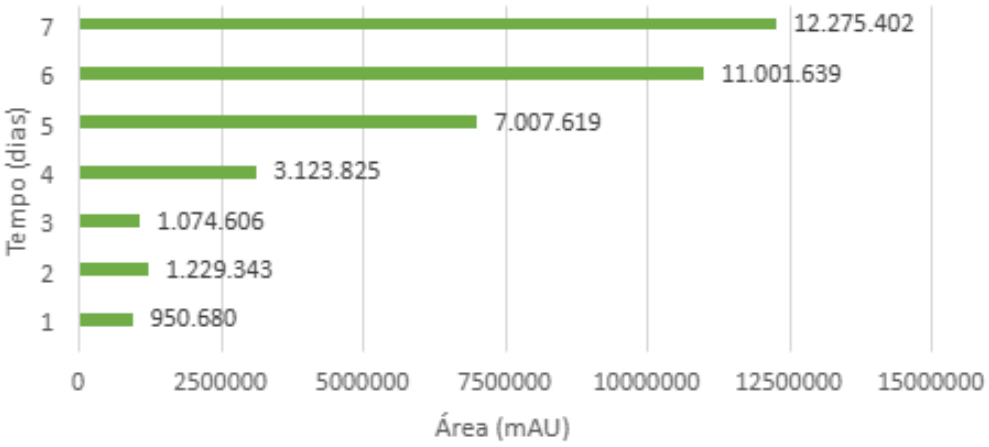
Highlights

Inorganic salts enhance 3-*O*-methylfuniconone production by 20-fold. Seven-day kinetics reveal peak yield on day 7. 3OMF displays significant inhibitory activity against*Helicobacter pylori*.

Resumo/Abstract

The imminence of multi-resistant pathogens and the high impact of chronic gastric diseases demand the discovery of new substances with pharmacological potential. The bacterium*Helicobacter pylori*stands out as the primary etiologic agent of gastritis, ulcers, and gastric neoplasms. Consequently, natural products biosynthesized by endophytic fungi have emerged as a promising source of bioactive and structurally complex specialized metabolites. This study aimed to modulate the metabolic profile of the endophytic fungus*Talaromyces pinophilus*J6, isolated from the leaves of*Euphorbia umbellata*, focusing on the production of the polyketide 3-*O*-methylfuniconone (3OMF), a compound typically isolated from the Talaromyces genus that possesses potent antimicrobial activities.To achieve this, the OSMAC (One Strain Many Compounds) strategy was applied by varying inorganic supplements in potato dextrose agar (PDA) medium across nine conditions. Ethyl acetate extracts were analyzed by High-Resolution Mass Spectrometry (UHPLC/ESI Q-Orbitrap), which revealed that cultivation supplemented with ammonium sulfate increased 3OMF production by approximately 20-fold. Seven-day monitoring under this condition demonstrated that 3OMF biosynthesis begins on the first day and reaches its maximum on the seventh day. Biological evaluation of 3OMF against*H. pylori*ATCC 43504 showed a Minimum Inhibitory Concentration (MIC) of 64 µg/mL and a Minimum Bactericidal Concentration (MBC) of 128 µg/mL. In comparison, amoxicillin (positive control) presented an MIC of 1 µg/mL and an MBC of 2 µg/mL. The results confirm that 3OMF biosynthesis increases progressively and that supplementation with inorganic salts is an efficient strategy to enhance the yield of metabolites with pharmacological potential.

1. KNOWLES, S. L. et al. Fungal–fungal co-culture: a primer for generating chemical diversity. Natural Product Reports, v. 39, n. 8, p. 1557–1573, 2022.



Production of 3-O-methylfunicone as a function of time

Optimization of Sustainable Resveratrol Extraction from Peanut Waste: Advancing Microwave, Ultrasound, and Dynamic NADES Methods

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Palavras Chave:*Arachis hypogaea,Microwave Assisted Extraction,Ultrasound Assisted Extraction,Dynamic Maceration Extraction,Waste valorization*

Highlights

NADES enable efficient and sustainable extraction of resveratrol from peanut waste. Lactic acid–glycerol and choline chloride–lactic acid NADES outperform ethanol-based extraction.

Resumo/Abstract

Brazil's agro-industrial sector generates substantial amounts of waste, highlighting the need for sustainable strategies to valorize these residues while reducing environmental impacts. In the state of São Paulo, peanuts (*Arachis hypogaea*) cultivation produces large quantities of agricultural by-products, such as shells, stems, roots, and leaves, which are rich in bioactive compounds, including resveratrol. In this study, green extraction strategies were evaluated for the efficient recovery of resveratrol from peanut residues using Microwave-Assisted Extraction (MAE), Ultrasound-Assisted Extraction (UAE), and Dynamic Maceration Extraction (DME) combined with Natural Deep Eutectic Solvents (NADES). Extraction parameters for each technique were optimized using Design of Experiments (DoE) to maximize resveratrol enrichment. For DME and UAE, lactic acid-glycerol (1:1, mol:mol) NADES exhibited the highest efficiencies, achieving 3.98- and 1.35-fold increases, respectively, compared to the best conventional ethanol-based reported in the literature. In MAE, choline chloride-lactic acid (1:2, mol:mol) NADES showed superior performance, with an efficiency 3.82 times higher than ethanol extraction. These results demonstrate that the interaction between the extraction technique and the physicochemical properties of the NADES employed strongly influences extraction efficiency. Therefore, the rational selection of the technique-solvent combination is crucial for developing a sustainable and high-efficiency process for the valorization of agro-industrial waste.

Agradecimentos/Acknowledgments

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OSMAC-driven elicitation of tetracycline-related metabolites in an ant-associated Pseudonocardia sp. revealed by metabolomics and molecular networking

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Palavras Chave:*: Natural products,tetracycline,Pseudonocardia,One Strain Many Compounds,metabolomics*

Highlights

Selected medium increased production of a putative tetracycline analogue
LC-MS/MS dereplication revealed known and potentially novel metabolites
Bioactive compounds isolated and under NMR analysis

Resumo/Abstract

This study aimed at the bioprospecting of bioactive metabolites with ecological and pharmaceutical relevance, using the actinobacterium*Pseudonocardia*sp. ICBG1860, a symbiont of attine ants, as a model system. Accordingly, the One Strain Many Compounds (OSMAC) approach was applied under the hypothesis that modulation of culture conditions could elicit silent biosynthetic pathways and induce the production of minor or previously unreported antimicrobial metabolites. Among the metabolites of interest, a putative tetracycline analogue previously detected at low concentrations (GRUNDMANN, 2023) was defined as the main target of this study.

The strain was cultivated in 11 different culture media. Solid cultures were extracted with ethyl acetate, whereas liquid cultures were processed using HP20 resin followed by acetone extraction. The resulting extracts were subjected to solid-phase extraction (SPE-C18) and analyzed by HPLC-DAD-ELSD. The D-mannitol–peptone agar medium induced the highest metabolic diversity compared to the other evaluated conditions. UV–Vis spectra suggested the presence of tetracycline analogues, while ELSD data revealed a significant increase in the production of the putative analogue.

Based on these results, large-scale cultivation was performed using the selected medium, followed by fractionation and LC-MS/MS analyses. The data were processed in MZmine and submitted to dereplication using the*Dictionary of Natural Products*and*Natural Products Atlas*databases, allowing the annotation of eight metabolites, namely: ravidomycin, paulomycin B, FCE24366, kigamicin C, sclerotide C, TAN-1518B and X, aestuaramide B, as well as several ions compatible with potentially new metabolites. The 75% MeOH fraction was prioritized for semi-preparative isolation by HPLC-DAD due to its observed bioactivity. To date, two compounds have been isolated and are currently under structural elucidation by ^{1}H and ^{13}C NMR spectroscopy (1D and 2D).

Agradecimentos/Acknowledgments

We acknowledge FAPESP, CNPq, and CAPES for financial support, and thank Prof. Dr. Mônica T. Pupo for her supervision, scientific guidance, and valuable discussions throughout this work.

Oxoaporphine Alkaloids Isolated from the Bark of Pseudoxandra leiophylla (Diels) R. E. Fries (Annonaceae)

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Palavras Chave:*Pseudoxandra leiophylla, Oxoaporphine alkaloids, Liriodenine, Atherospermidine, Chemophenetics*

Highlights

1. Two oxoaporphine alkaloids were isolated from the bark of Pseudoxandra leiophylla.
2. First report in this species.
3. Expands the chemophenetic knowledge of the genus Pseudoxandra.

Resumo/Abstract

Pseudoxandra leiophylla (Diels) R. E. Fries is a species of the Annonaceae family, popularly known as “envira-preta” and “envira-roxa”, native to the Amazon region and distributed in Brazil, Colombia, and Venezuela. Its accepted synonym is Pseudoxandra coriacea R. E. Fries. According to the literature, only one phytochemical study has been reported for this species, describing the isolation of alkaloids, terpenes, and lignoids from the alkaloid fraction obtained after acid-base treatment of the methanolic leaf extract, aimed at cytotoxic activity evaluation and conducted by the GEQBiom research group.[1] In the present study, a phytochemical investigation of the alkaloid fraction obtained from the methanolic extract of the bark of P. leiophylla was carried out using classical chromatographic techniques, including column chromatography (CC) and thin-layer chromatography (TLC). This approach initially led to the isolation of two alkaloids (1 and 2). Structural elucidation was achieved through spectroscopic analyses (1H and 13C NMR, 1D and 2D) and mass spectrometry (MS), allowing the identification of the oxoaporphine alkaloids liriodenine (1) and atherospermidine (2).[2] These alkaloids are reported for the first time in the bark of P. leiophylla. While liriodenine had previously been described in the leaves of this species, atherospermidine is reported here for the first time in the genus Pseudoxandra. These findings contribute to the chemophenetic knowledge of P. leiophylla and its genus, which remains poorly studied according to the available literature.

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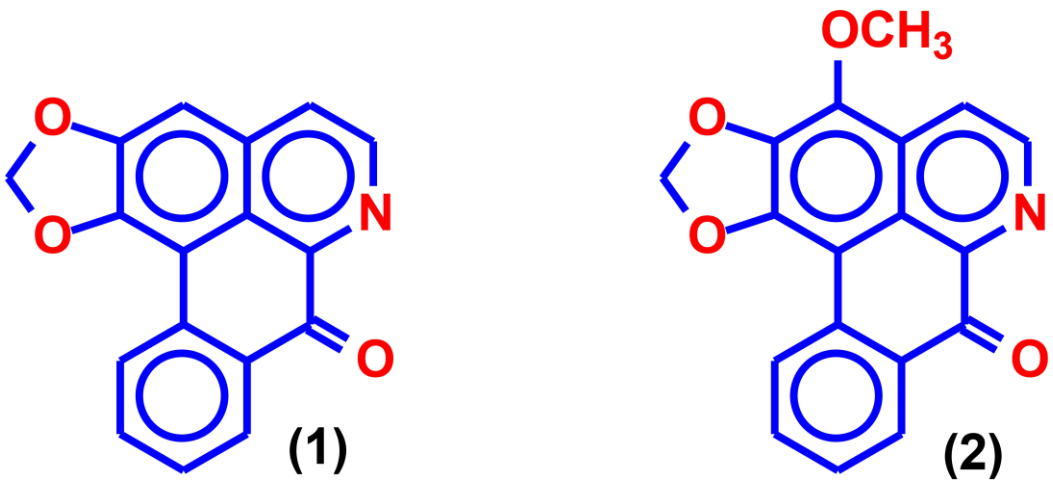


Figure 1. Structure of isolated oxoaporphine alkaloids liriodenine (1) and atherospermidine (2).

Agradecimentos/Acknowledgments

The authors acknowledge CAPES and CNPq (Grant No. 306335/2023-9; Pró-Amazônia/CNPq Grant No. 445615/2024-9) for financial support, and CA/CAM/UFAM for NMR and MS analyses.

Patent review on essential oils from Citrus spp. applied to the treatment of leishmaniasis

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Palavras Chave:*Leishmaniasis, Treatment, Patents, Essential Oil.,Essential oils, Citrus spp., Leishmaniasis, Natural products, Patents.*

Highlights

New technologies based on essential oils for the treatment of leishmaniasis.

Resumo/Abstract

Leishmaniasis is a neglected parasitic infectious disease caused by protozoa of the genus*Leishmania*. Current treatments are constrained by toxicity, adverse effects, and invasive administration routes. Consequently, natural products have been explored as therapeutic alternatives, with particular attention to essential oils from*Citrus*species, which are widely produced in Brazil. The primary constituent of*Citrus sinensis*essential oil is d-limonene, a monoterpene found in citrus fruit peels, recognized for its solvent properties and potential as a carrier for bioactive compounds such as lapachol. This study presents a patent review of technologies for alternative treatments of leishmaniasis using essential oils from*Citrus*species. The review identified four relevant patents involving*Citrus sinensis*(orange),*Citrus limon*(lemon), and*Citrus reticulata*(tangerine). The patented technologies include formulations with additional plant extracts, strategies to enhance biological activity, and microemulsion systems designed to increase leishmanicidal efficacy. Essential oils from*Citrusspp.*are predominantly used in combination with other plant extracts to exploit synergistic effects among secondary metabolites. This strategy underscores the potential of citrus agro-industrial waste-derived essential oils as sustainable sources of bioactive compounds, with broad applicability in the development of novel pharmaceutical technologies.

Agradecimentos/Acknowledgments

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Photoprotective and antioxidant emulgel Formulation containing 70% tocotrienol enriched fraction produced from Bixa orellana L.

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Palavras Chave:*Sunscreen agents; antioxidants; tocotrienols; Bixa orellana; photoprotection*

Highlights

Tocotrienol fraction from bixin industrial by-product with potent antioxidant activity, with synergistic SPF booster effect, meeting ANVISA'S formulation strability criteria.

Resumo/Abstract

This study developed a photoprotective and antioxidant cosmetic emulgel using a 70% tocotrienol-enriched fraction, a byproduct of bixin dye production from*Bixa orellana*L., as the active ingredient. The formulation contained 5% of the tocotrienol fraction, 3.5% octyl methoxycinnamate, and 2% benzophenone-3. Stability was assessed through preliminary and accelerated tests (up to 90 days at room temperature and 40 ± 2 °C), with monitoring of macroscopic characteristics, pH, viscosity, density, tocotrienol content, antioxidant activity (FRAP and DPPH assays), and in vitro Sun Protection Factor (SPF). Physicochemical parameters remained within ANVISA stability criteria (variation ≤ 10%). The tocotrienol fraction exhibited an SPF-boosting effect, increasing the SPF from 4.83 (blank) to 6.13 (active) initially, and from 4.13 to 5.67 after 90 days. Although total tocotrienol content gradually decreased over time (from 3.41% to 2.85%), antioxidant activity remained stable throughout the study. These findings demonstrate that the 70% tocotrienol-enriched fraction is a viable multifunctional active ingredient for sunscreen formulations, adding value to the industrial production chain and supporting sustainable development goals.

Agradecimentos/Acknowledgments

The authors thank the São Paulo Research Foundation (FAPESP) for financial support (Grant 2024/02257-3) and the Faculty of Pharmaceutical Sciences at UNICAMP.

PHYTOCHEMICAL CHARACTERIZATION AND ANTIOXIDANT ACTIVITY OF *Trichilia sylvatica* C. DC. LEAVES

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Palavras Chave:*Trichilia silvatica; chromatographic techniques; antioxidant activity; phenolic acids,Trichilia silvatica; chromatographic technics; antioxidant capacity; phenolic acids.*

Highlights

Phytochemical profiling revealed caffeic and quinic acids and rutin in extracts from*Trichilia silvatica*.

Chemical composition correlated with antioxidant and predicted anti-inflammatory potential.

Resumo/Abstract

Trichilia silvatica, popularly known as*catiguá*,*catiguá-branco*,*cutia-vermelha*and*rosa-branca*, is traditionally used to treat rheumatism. This study aimed to characterize the hydroethanolic extract from*T. silvatica*leaves (EHTS) and its ethyl acetate fraction (EHTS-EtOAc), as well as to evaluate their antioxidant capacity in vitro. TLC, HPLC-PDA, and UPLC-PDA-ESI-MS were used for chemical characterization. TLC analysis revealed the presence of tannins, flavonoids and antocyanins in both samples. Analysis by UPLC-PDA-ESI-MS allowed the putative identification of caffeic and quinic acids, rutin, kaempferol-3-rutinoside and a di-*O*-caffeoylquinic acid. Notably, caffeic acid was detected by all chromatographic techniques employed. The amounts of polyphenols, flavonoids and antocianins were spectrophotometrically determined. EHTS showed 241.17 ± 3.16 mg of equivalents of pyrogallol (EP), 31.53 ± 0.14 mg of equivalents of quercetin (EQ) and 229,11 ± 4.74 mg of equivalents of cyanidin(EC)/ g of dry weight. EHTS-EtOAc fraction had lower levels of polyphenols (157.65 ± 2.20 mg EP/g) and flavonoids (19.40 ± 0.47 mg EQ/g) while antocyanins (534.47 ± 5.98 mg EC/g) were higher than those observed for EHTS. The antioxidant capacity was evaluated using DPPH scavenging, β-carotene/linoleic acid co-oxidation and TBARS assays EHTS showed significant capacity of DPPH scavenging (IC_{50} = 5.10 ± 0.23 µg/mL) and moderate prevention of β-carotene/linoleic acid co-oxidation (IC_{50} = 116.87 ± 11.22 µg/mL). In contrast, the EHTS-EtOAc fraction exhibited lower antioxidant capacity, with DPPH scavenging (IC_{50} = 59.77 ± 2.81 µg/mL). These findings suggest that EHTS has antioxidant potential, which may contribute to its traditional use. However, further studies are needed to confirm this results. In silico prediction of caffeic acid indicated the potential antioxidant and anti-inflammatory activities, as well as possible applications of immunologic, vascular, methabolic and neurologic disorders.

Agradecimentos/Acknowledgments

The authors are grateful to FAPEMIG by financial support (Process APQ-00373-21) and the fellowship of VL Almeida (BIP-00213-24).

Phytochemical profile and antiparasitic activity of Pereskia aculeata and P. grandifolia fractions against Leishmania, Trypanosoma, and Schistosoma.

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Palavras Chave:*Pereskia aculeata; Pereskia grandifolia; phytochemical profile; antiparasitic activity; neglected parasitic diseases.*

Highlights

Fractions of*Pereskia aculeata*and*P.grandifolia*are evaluated for their phytochemical profile, leishmanicidal, trypanocidal, and schistosomicidal activities, and cytotoxicity.

Resumo/Abstract

Neglected parasitic diseases, including leishmaniasis, schistosomiasis, and Chagas disease, remain major public health challenges, particularly in developing countries, underscoring the urgent need for novel therapeutic agents with improved efficacy and reduced toxicity. In this context, plant species of the genus*Pereskia*have attracted increasing scientific attention due to their promising biological properties. This study aimed to investigate the phytochemical profile and the leishmanicidal, schistosomicidal, and trypanocidal activities of fractions obtained from leaf extracts of*Pereskia aculeata Miller*and*Pereskia grandifolia Haw.*Dried leaves were ground and subjected to maceration, followed by filtration and solvent evaporation to obtain crude extracts, which were subsequently fractionated by liquid–liquid partitioning using solvents of increasing polarity. The metabolic profiles of the fractions were characterized by high-performance liquid chromatography coupled to diode-array detection (HPLC-DAD) and by colorimetric assays for the identification of secondary metabolite classes. Leishmanicidal activity was evaluated in vitro against*Leishmania amazonensis,*while schistosomicidal and trypanocidal activities were assessed against*Schistosoma mansoni*and*Trypanosoma cruzi,*respectively. Cytotoxicity was determined in host cells, and cell viability was assessed using the XTT assay. The results allow the identification of fractions exhibiting significant antiparasitic activity combined with low cytotoxicity, contributing to the discovery of bioactive plant-derived compounds. Overall, these findings highlight*Pereskia aculeata*and*Pereskia grandifolia*as promising sources of lead compounds for the development of new therapies targeting neglected parasitic diseases.

Agradecimentos/Acknowledgments

The authors acknowledge CAPES (Finance Code 001), FAPESP, CNPq (Process Number 302992/2022-7) and Unifran for the support.

Phytochemical Profiling and Antiparasitic Potential of Pyrostegia venusta (Bignoniaceae) against Neglected Tropical Diseases

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Palavras Chave:*Bignoniaceae,Dereplication,HPLC-DAD,Antiparasitic activity,NTDs*

Highlights

*P. venusta*profiling reveals bioactive fractions against NTDs, identifying it as a source of antiparasitic leads and expanding Bignoniaceae knowledge.

Resumo/Abstract

Natural products remain a major source of chemical scaffolds for drug discovery, particularly for neglected tropical diseases (NTDs).*Pyrostegia venusta*(Bignoniaceae), widely distributed in Brazil, possesses relevant ethnopharmacological uses; however, the correlation between its chemical profile and antiparasitic activity requires further investigation. This study aimed to prioritize bioactive fractions of*P. venusta*through a dereplication strategy combining phytochemical screening and biological assays. Aerial parts were collected in Franca, SP (Sept/2025), a voucher specimen was deposited at the Herbarium Uberlandense (HUFU 89686) and the research was registered in SisGen under code AA65004. The dried material underwent ethanolic extraction, followed by liquid-liquid partitioning with solvents of increasing polarity (hexane, dichloromethane, chloroform, and ethyl acetate). HPLC-DAD analysis and colorimetric assays were performed to characterize the metabolic profile. Results indicated a significant content of phenolic compounds and flavonoids, corroborated by UV absorption patterns. Bioassay-guided fractionation is prioritizing fractions with activity against*Trypanosoma cruzi*and*Leishmania*sp., guiding the isolation of active metabolites, also using chromatographic and spectroscopic techniques (NMR and MS). These findings reinforce the bioactive potential of*P. venusta*, highlighting the species as a promising source of scaffolds for anti-NTD drug development.

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Phytochemical profiling of the ornamental plant Stromanthe thalia by HPLC–QTOF-MS

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Palavras Chave:*Stromanthe thalia; phytochemical profile; phenolic compounds; HPLC–QTOF-MS; ornamental plant,Stromanthe thalia; phytochemical profile; phenolic compounds; HPLC–QTOF-MS; ornamental plant*

Highlights

Phytochemical profiling of the ornamental plant*Stromanthe thalia*
Aqueous acidic extraction favors phenolic compound detection
Phenolic acids and flavonoids dominate the chemical profile

Resumo/Abstract

Stromanthe thalia(Vell.) J.M.A.Braga is an ornamental plant, belonging to the family Marantaceae. Despite its widespread ornamental use, studies addressing its phytochemical characterization remain scarce, particularly with respect to its phenolic composition. In this study, the phytochemical profile of aqueous leaf extracts of*S. thalia*was investigated using high-performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (HPLC–QTOF-MS), operating in both positive and negative ionization modes under an exploratory approach. Leaf samples were extracted with water containing 0.1% formic acid for 48 h under magnetic stirring, followed by a 10-min ultrasonic bath treatment at 30 °C. The resulting extracts were analyzed by HPLC coupled to diode array detection (DAD) and QTOF-MS. Compound annotation was based on accurate mass measurements, retention times, isotopic patterns, and comparison with data reported in the literature. The results revealed a phytochemical profile dominated by phenolic acids and flavonoids. In negative ion mode, hydroxycinnamic acid derivatives, such as caffeic acid (m/z 179), caffeoylquinic acids (m/z 353), dicaffeoylquinic acids (m/z 515), and related shikimate conjugates were clearly detected, along with organic acids. Flavonoids and flavonoid glycosides, including quercetin (m/z 303), myricetin (m/z 317), vitexin (m/z 448), quercitrin (m/z 447), and quercetin rutinosides, were observed in both ionization modes. Positive ion mode additionally facilitated the detection of flavonoid aglycones and glycosylated derivatives, such as quercetin (m/z 303), kaempferol-3-O-rutinoside, isovitexin (m/z 433), as well as anthocyanin-related compounds. Overall, the combined HPLC–QTOF-MS approach provided a robust phytochemical characterization of*S. thalia*, highlighting its richness in phenolic compounds and supporting further investigations into the chemical diversity and potential bioactivity of this species.

Agradecimentos/Acknowledgments

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PHYTOCHEMICAL STUDY AND EVALUATION OF THE ANTI-INFLAMMATORY AND ANTIFUNGAL ACTIVITY OF Luehea divaricata Mart. (MALVACEAE)

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Palavras Chave:*Luehea divaricata Mart., fitoterápicos, flavonoides.*

Highlights

*Luehea divaricata*showed antioxidant, antifungal, and anti-inflammatory potential with low cytotoxicity.

First study from Maranhão supports its traditional use and phytotherapeutic potential.

Resumo/Abstract

The use of medicinal plants in Brazil is rooted in traditional knowledge from Indigenous, African, and European cultures and remains an important therapeutic resource.*Luehea divaricata*(“açoita-cavalo”) is traditionally used to treat inflammation, ulcers, dysentery, and infections, motivating studies on its pharmacological potential. This research identified and characterized secondary metabolites from leaf extracts and evaluated their antioxidant, antifungal, anti-inflammatory, and cytotoxic activities. Sequential extraction (hexane, ethyl acetate, and methanol) was followed by purification (HPLC) and structural analysis (LC–MS and NMR), identifying flavonoids such as kaempferol-7-O-glycoside, genistein derivatives, and quercetin-3-O-glycoside. The methanolic extract showed the highest antioxidant activity in the DPPH assay, while ethyl acetate and methanol extracts inhibited*Fusarium*growth. Anti-inflammatory assays demonstrated reduced nitric oxide production, especially with the ethyl acetate and hexane extracts, both showing low cytotoxicity. This first chemical and biological investigation of*L. divaricata*from Maranhão highlights its potential as a source of bioactive flavonoids with antioxidant, antifungal, and anti-inflammatory properties, supporting its traditional use and relevance for phytotherapeutic development

Agradecimentos/Acknowledgments

I am grateful to God, to my advisors Alan Bezerra and Antônio Filho, to FAPEMA, IFMA, and to all collaborators for their support and contributions to this work.

Phytochemical study of roots of Mabea paniculata (Euphorbiaceae)

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Palavras Chave:*Euphorbiaceae, Mabea paniculata, secondary metabolites, norditerpene,Euphorbiaceae,Mabea paniculata,secondary metabolites,norditerpene*

Highlights

First phytochemical study of the*M. paniculata*.
Four phytosterols, two diterpenes and one alkaloid known from*M. paniculata.*
Isolation and identification of a new nor-diterpene present in the species.

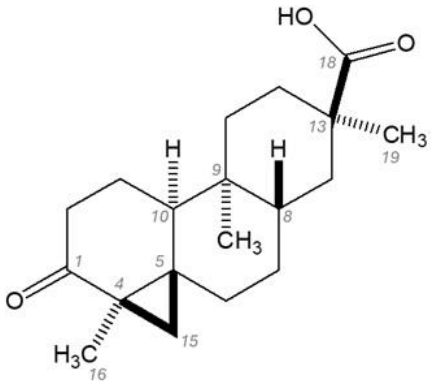
Resumo/Abstract

The genus*Mabea*Aubl., belonging to the Euphorbiaceae family, comprises about 50 species distributed in Central and South America, showing greater diversity in the Amazon region. In Brazil, it is represented by about 25 species, 5 of which are endemic [1]. To date, only three species of this genus have been chemically studied. In order to expand the study of this genus, the present work aims to carry out the phytochemical study of the roots of the species*Mabea paniculata*Spruce ex Benth. This species occurs from Mato Grosso do Sul to Pará [2] and there are still no reports in the literature on its phytochemical study. For this study, plant material was collected in Pantanal region, in Santo Antônio do Leverger – MT. The exsiccata was deposited and registered in the herbarium of the Federal University of Mato Grosso (no. 44467) and in SisGen (A3831B0). The roots were dried and subjected to extraction with methanol through cold maceration. The crude extract was dissolved in a methanol:water mixture (7:3) and partitioned with organic solvents in increasing order of polarity until complete extraction: hexane, dichloromethane, and ethyl acetate, generating 4 different fractions. The less polar fractions were subjected to separation by silica gel column chromatography. From subfractions of the hexane fraction, it was possible to identify 4 known substances in mixture: β-sitosterol, stigmasterol, stigmasta-3,5-dien-7-one, and campesterol. The study with the dichloromethane fraction led to the isolation and identification of a new nor-diterpene, and a mixture containing two derivatives/precursors of this terpene and one indole alkaloid. The structural elucidation of these substances was carried out using one- and two-dimensional NMR, mass spectrometry and DC techniques, comparing their data with literature models [3].

[1] SILVA et al. Flora da Bahia:*Mabea*(Euphorbiaceae) 2023.

[2] CORDEIRO et al.*Mabea*in Flora e Funga do Brasil 2025.

[3] RAHMAN et al. Tetrahedron 1986.



New nor-diterpene named 4R,5R,8S,9S,10S,13R-3-keto-18-norditerpenoic acid

Agradecimentos/Acknowledgments

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plantMASST: a mass spectrometry tool for mining public datasets from plants

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Palavras Chave:*Plant metabolomics, Tandem mass spectrometry, Plant reference database*

Highlights

plantMASST enables the taxonomic exploration of plant-derived molecules, being of great value for drug discovery, chemotaxonomy, and dietary patterns.

Resumo/Abstract

Plants produce diverse specialized metabolites, many of which have been used for drug development. Despite their importance, the identification of plant-derived molecules and the elucidation of their biological roles and biosynthetic pathways remain challenging. Addressing this gap requires mass spectrometry (MS) tools tailored to the plant metabolome. Here, we introduce plantMASST, a mass spectrometry search tool that leverages a curated reference database of plant extracts. Publicly available LC-MS/MS data deposited in GNPS/MassIVE (https://massive.ucsd.edu/) were systematically organized and metadata-curated to generate a taxonomically structured reference dataset. Query MS/MS spectra are searched against this reference space, enabling contextualization of both known and previously uncharacterized metabolites within the plant kingdom. plantMASST is available as a Python script and as a standalone web interface integrated into the GNPS environment (https://masst.gnps2.org/plantmasst/). The current plantMASST reference database comprises over 42,000 LC-MS/MS files, 128 million MS/MS spectra, and represents 318 plant families, 1,727 genera, and 3,568 species. Using plantMASST, we identify previously unrecognized producer species for known bioactive metabolites, including expanded taxonomic distributions of compounds such as moroidin and piperlongumine, supported by MS/MS matching and orthogonal validation. In addition, analog searches enable discovery of structurally related natural products and facilitate biosynthetic pathway inference when integrated with transcriptomic and genomic data. Beyond plant metabolomics, plantMASST can be applied to human datasets to detect plant-derived metabolites and empirically assess dietary exposure patterns. Together, these results establish plantMASST as a scalable framework for mapping plant metabolite distributions and advancing discovery in drug discovery, nutrition, and chemical ecology.



Schematic overview of plantMASST infrastructure.

Agradecimentos/Acknowledgments

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Production of betulinic acid in calli cultured from Abarema cochliacarpos seedlings

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Palavras Chave:*Inflammation,triterpene,tissue culture*

Highlights

*Abarema cochliacarpos*is a Leguminosae with anti-inflammatory properties. Callus cultures established from seedling explants of this plant produced betulinic acid, not found in leaves and bark.

Resumo/Abstract

Barbatimão or ingá negro are the common names of*Abarema cochliacarpos*, a Leguminosae species traditionally used for medicinal purposes in southeastern and northeastern Brazil. This Brazilian native plant occurs mainly along the coasts of Rio de Janeiro and Espírito Santo and in inland and coastal areas of Bahia. Stem bark preparations, including teas and tinctures, are employed to treat inflammation, promote wound healing, relieve pain, and exhibit analgesic effects.
To establish*in vitro*cultivation and compare the chemical composition with soil-grown plants, seeds were disinfected and germinated on Murashige and Skoog (MS) medium to obtain seedlings. After five months, rachis, root, leaflet, and hypocotyl explants were cultured separately on MS medium supplemented with 2.24 µM 2,4-D to induce callus formation. Calli were lyophilized, extracted with methanol, and analyzed chromatographically. Thin-layer chromatography revealed a major low-polarity compound soluble in dichloromethane and hexane/ethyl acetate mixtures. The extract was fractionated by silica gel column chromatography, and the main compound was purified and characterized by one- and two-dimensional ^{1}H and ^{13}C NMR. Careful analysis of the isolated compound's NMR spectra and comparison with literature data identified it as betulinic acid. This triterpene, known for antitumoral and anti-inflammatory activities, was not detected in metabolomic analyses of leaf and branch extracts, suggesting a distinct metabolism operating in the species' callus tissues.

Agradecimentos/Acknowledgments

The authors would like to thank CNPq and FAPERJ for the scholarships granted.

Prospecção de inibidores naturais das enzimas elastase e tirosinase em extratos vegetais do Cerrado.

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Palavras Chave:*Plantas do Cerrado, inibidores, tirosinase, elastase.*

Highlights

Cerrado plant extracts showed elastase and tyrosinase inhibition. Lippia origanoides reached 92% inhibition, while luteolin and naringenin showed about 50%, indicating promising cosmetic potential.

Resumo/Abstract

A biodiversidade brasileira representa uma fonte estratégica de compostos bioativos com potencial aplicação cosmética, especialmente aqueles relacionados à prevenção do envelhecimento cutâneo e da hiperpigmentação. Este trabalho investigou a atividade inibitória de extratos etanólicos de plantas do Cerrado frente às enzimas elastase e tirosinase, alvos diretamente associados a processos de degradação de matriz extracelular e melanogênese. Os ensaios in vitro foram conduzidos a 100 µg/mL, utilizando L-DOPA e Suc-Ala_3-pNA como substratos para tirosinase e elastase, respectivamente. A atividade enzimática foi monitorada por espectrofotometria, acompanhando a formação de L-dopaquinona (475 nm) e p-nitroanilida (410 nm). Entre as espécies avaliadas, Lippiaoriganoides Kunth (Verbenaceae) aparesentou 92% de inibição da tirosinase, sendo selecionada para estudo bioguiado. A desreplicação permitiu anotar compostos majoritários, e padrões comerciais foram testados a 100 µM: luteolina (1), naringenina (2), apigenina (3), floretina (4) e luteolina glicosilada (5). Luteolina e naringeninaapresentaram cerca de 50% de inibição da tirosinase, sugerindo que tais flavonoides contribuem para a bioatividade observada no extrato. Os resultados evidenciam o potencial de espécies vegetais como fontes de inibidores naturais, destacando a relevância de abordagens bioguiadas para a identificação de candidatos com possível aplicabilidade em formulações cosméticas voltadas ao cuidado da pele. Referência: Vieira, J. L. Análise química de L. origanoides e prospecção de ativos para potencial uso cosmético. Dissertação (Mestrado em Química) – Instituto de Química, Universidade Federal de Catalão, 2025.

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Quantificação de Fenóis Totais e Atividade Antioxidante de Solanum paniculatum L (Jurubeba)

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Palavras Chave:*medicinal plant,total phenolic content,antioxidant activity,metabolomic assay*

Highlights

Valorização do conhecimento quilombola por meio de ensaios espectrofotométricos de extratos de Jurubeba. Os extratos foliares apresentaram alta atividade antioxidante e alto teor de fenóis totais.

Resumo/Abstract

Solanum paniculatum L., conhecida popularmente como Jurubeba, é utilizada na medicina tradicional da Comunidade de Três Lagoas, Amargosa-BA, no tratamento da tosse causada pela gripe[1]. Pertencente à família*Solanaceae*, o gênero apresenta mais de 1.000 espécies, distribuídas no Nordeste Brasileiro. Estudos reportam a presença de diversos metabólitos secundários[2] e Atividade Antioxidante (AA) em extratos aquosos e etanólicos de espécimes cultivadas em outras regiões do Brasil. Na perspectiva de validar o uso popular, extratos foliar e caulinar em metanol, acetato de etila e hexano foram submetidos às análises espectrofotométricas pelo método do DPPH, na determinação da AA a 515 nm, e pelo método Folin-Ciocalteu a 725 nm, na quantificação de Fenóis Totais (FT). As análises foram realizadas em triplicata e o ácido gálico foi utilizado como padrão. Os extratos foliares em metanol e acetato foram os que apresentaram maior AA e concentração de FT (Tabela 1). Os dados da AA encontrados atestam com a literatura, que apresenta o IC50 (33,46 - 434,55 $\mu g.mL^{-1}$)[2]. A AA geralmente está associada a um maior valor de FT, no entanto, a quantificação por Folin-Ciocalteu sofre interferência ao detectar substâncias não fenólicas[3], resultando em dados não lineares, como o observado para o extrato metanólico do caule. A concentração de metabólitos associados à AA varia com o habitat e condições de cultivo. A alta concentração de FT e da AA observadas nos extratos contribuem para a neutralização de radicais livres produzidos durante as infecções virais, tornando-os promissores no tratamento de enfermidades, corroborando o uso em Três Lagoas. Os dados encontrados além de valorizar o conhecimento tradicional, contribuem para a preservação da biodiversidade local.

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Tabela 1- Resultados da atividade antioxidante e quantificação de fenóis dos extratos de *S. Paniculatum L.*

Extratos	IC_{50} [a]($\mu g.mL^{-1}$) ± DP	Teor de fenóis totais (mg EAG.g^{-1})[b] ± DP
Foliar em Metanol	153,81 ± 3,75	283,98 ± 5,33
Caulinar em Metanol	527,84 ± 18,74	258,79 ± 1,07
Foliar em Acetato de Etila	243,66 ± 22,63	264,58 ± 8,47
Caulinar em Acetato de Etila	218,77 ± 4,58	237,75 ± 1,98
Foliar em Hexano	408,90 ± 7,80	159,88 ± 2,71
Caulinar em Hexano	> 1000,00	163,38 ± 13,67
Ácido Gálico	2,19 ± 0,053	—

a-concentração mínima para inibir 50% do radical DPPH; b-mg equivalente de padrão por g de extrato

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Laboratório de Biotecnologia e Química de Microrganismos da UNIVERSIDADE FEDERAL DA BAHIA (LBQM)

Schizotrins B–E: New Cyclic Peptides from a Brazilian Cyanobacterium with Antibacterial Activity

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Palavras Chave:*Antimicrobial,Cyanobacteria,Brazilian biodiversity,Natural Products,Phormidium*

Highlights

Discovery of four peptides from*Phormidium*sp. Structural elucidation employed NMR spectroscopy, mass spectrometry, and Marfey's analysis Major compound showed bioactivity against*Bacillus anthracis*

Resumo/Abstract

Brazilian biodiversity represents one of the most promising sources for the discovery of natural products with biotechnological potential. Nevertheless, within the taxonomic group of cyanobacteria, especially those of Brazilian origin, the search for new molecules remains largely underexplored. Here, we report the discovery, structural elucidation, and antimicrobial profile of four new cyclic peptides belonging to the schizotrin family, isolated from a*Phormidium*sp. strain and designated schizotrins B–E. These compounds were obtained from 40-L cultures and characterized by one- and two-dimensional NMR spectroscopy, as well as mass spectrometry. The relative stereochemical configurations of the structures were determined by a combination of Marfey's analysis and two-dimensional NMR experiments such as HSQC-TOCSY and ROESY. Antimicrobial assays performed against*Bacillus anthracis*demonstrated complete growth inhibition at 6.25 µg/mL for the major compound. This finding highlights the potential of Brazilian cyanobacteria as a valuable source of novel antibiotics.

Agradecimentos/Acknowledgments

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Screening of Antioxidant Secondary Metabolites Produced by Penicillium sp. CML-3020

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Palavras Chave:*Secondary metabolites; Antioxidant activity; Phenalenones; Penicillium.*

Highlights

Phenalenones with antioxidant activity were identified in the new species Penicillium sp. CML-3020 during the screening of secondary metabolites.

Resumo/Abstract

The exploration of secondary metabolites produced by poorly studied species of the genus*Penicillium*represents a relevant strategy for the discovery of new compounds with antioxidant activity.*Penicillium*sp. CML-3020 corresponds to a new species isolated from Atlantic Forest leaf litter and remains scarcely investigated from metabolomic and biological perspectives. Phylogenetic analyses indicate that this strain is closely related to*P. herquei*, a species known for the production of phenalenones, a class of polyketides characterized by structural diversity and a wide range of reported biological activities, including antioxidant effects.

In this study, the crude extract and chromatographic fractions were evaluated for antioxidant capacity using the DPPH radical scavenging assay. Metabolomic profiling revealed the presence of phenalenone-type metabolites, from which three compounds were isolated and identified as penicifenalin E (1), sclerodine (2), and desmethyl-1235 (3). These metabolites were subjected to biological assays to assess their antioxidant activity. The results demonstrated that all three isolated compounds exhibited antioxidant activity, highlighting the potential of this new fungal species as a source of secondary metabolites of interest in Natural Products Chemistry. Therefore,*Penicillium*sp. CML-3020 warrants further investigation regarding its metabolic production, as it represents a new species from Brazilian biodiversity capable of producing antioxidant secondary metabolites.

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Secondary Metabolites Produced by the Marine-Derived Fungus Nigrograna sp.

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Palavras Chave:*Polyketides, marine fungus, Plasmodium, malaria*

Highlights

Nigrogranatides A–H were isolated and identified from the growth medium of Nigrograna sp., along with nitrogenated compounds. Two metabolites displayed moderated anti-plasmodial activity.

Resumo/Abstract

Fungi are distributed across terrestrial, freshwater, and marine environments. Their ease of cultivation allows large-scale production of secondary metabolites, many of which are biologically active. The genus Nigrograna, includes 37 registered species and produces compounds such as volatile polyenes and ergosterol derivatives. In this study, Nigrograna sp. M-13, isolated from the viscera of a brittle star collected in Guarapari, was cultivated in PDB. Isolation, characterization and biological evaluation of its metabolites, resulted in the discovery of ten new compounds, including bisalternariol, 6-methoxy-1,9-dimethylguanine and polyketides with novel skeletons named nigrogranetides A–H.

Investigation of the EtOAc-soluble fraction was performed after liquid-liquid partition of the culture broth. The MeOH/EtOAc (1:1, v/v) extract of the mycelium of Nigrograna sp. was also investigated. Isolation was performed by a series of chromatographic steps, to yield eight novel polyketides with unprecedented carbon skeletons, a new hydroquinone dimer, an undescribed guanine derivative, along with seven known metabolites. The planar structures of all compounds were determined based on spectroscopic and spectrometric data. The relative configurations were established by analyses of NOESY experiments. Electronic circular dichroism, together with theoretical NMR calculations and NOESY data, allowed the assignment of the absolute configurations of nigrogranatides E–H.

Among the compounds isolated from the strain M13, two exhibited moderate activity against Plasmodium falciparum 3D7 strain (chloroquine sensitive), with IC_{50} values of 7.1 µM and 4.9 µM, respectively. These findings indicate that nigrogranatides derivatives are hit candidates with attractive antiplasmodial activities for inhibitor development.

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Selective Cytotoxic Activity of Ethanolic Extracts from Leaves and Flowers of Alpinia purpurata against Human Cancer Cell Lines

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Palavras Chave:*anticancer,extracts,Alpinia purpurata,selectivity*

Highlights

*Alpinia purpurata*ethanolic extracts show pronounced selective cytotoxicity toward leukemia cells while sparing non-neoplastic cells.

Resumo/Abstract

Cancer comprises a heterogeneous group of diseases driven by genetic and epigenetic alterations that result in uncontrolled cell proliferation, resistance to programmed cell death, and disruption of tissue homeostasis, representing one of the leading causes of mortality worldwide. The search for new anticancer agents has highlighted plant-derived flavonoids and polyphenols due to their selective cytotoxic effects and reduced toxicity toward non-neoplastic cells. In this context, the present study investigated the cytotoxic activity and selectivity of ethanolic extracts obtained from the leaves (AZFA) and flowers (AZFR) of*Alpinia purpurata*. Plant material was collected in the state of Pará, Brazil, botanically identified (SISGEN A8B39D2), and subjected to ethanolic extraction. Cytotoxic activity was evaluated in human tumor cell lines—NALM-6 (leukemia), T98 (glioblastoma), and U2OS (osteosarcoma)—as well as in non-neoplastic HEK-293 cells using a colorimetric viability assay, allowing the determination of IC_{50} values and selectivity indices (SI). Both extracts exhibited selective cytotoxic activity, with NALM-6 cells showing the highest sensitivity. AZFA and AZFR showed strong cytotoxicity toward NALM-6 leukemia cells (IC_{50} = 10.8 and 15.9 µg/mL; SI = 18.1 and 12.6, respectively), moderate activity against T98 and U2OS cells, and minimal toxicity in HEK-293 cells (IC_{50} ≥ 195.6 µg/mL). This profile is consistent with the presence of flavonoids reported as bioactive against cancer cells, including cyanidin-3-O-rutinoside, rutin, quercetin, and isorhamnetin-3-O-rutinoside, as well as flavones and methoxylated flavonoids associated with cell cycle arrest, apoptosis induction, and modulation of tumor-related signaling pathways. These findings demonstrate that*Alpinia purpurata*extracts exhibit pronounced selective cytotoxicity, particularly against leukemia cells, supporting their potential as a source of safer anticancer agents.

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Solvent design matters: NADES–MAE extraction links flavonoid recovery to in vivo antioxidant performance

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Palavras Chave:*Drosophila melanogaster, in vivo antioxidant activity, Biomass valorization*

Highlights

NADES with MAE enhance flavonoid extraction from sugarcane bagasse and outperform methanol in yield and safety. Improved extraction efficiency translates into enhanced*in vivo*antioxidant responses.

Resumo/Abstract

Sugarcane bagasse is a promising source of antioxidant flavonoids, however, its efficient and safe exploitation strongly depends on the extraction medium. In this study, ten natural deep eutectic solvents (NADES) were evaluated for the extraction of flavonoids from sugarcane bagasse using microwave-assisted extraction (MAE), with performance was compared to conventional methanolic extraction. Beyond extraction efficiency, the biological effects of the resulting extracts were assessed in*Drosophila melanogaster*through longevity and locomotor performance assays.

Nine out of the ten NADES systems produced higher flavonoid recoveries than methanol, highlighting the role of NADES hydrogen-bonding networks in enhancing polyphenol solubilization. Among them, the choline chloride:lactic acid system exhibited the highest extraction efficiency. Importantlydifferences in extraction performance were reflected in distinct biological outcomes. Flies exposed to the choline chloride:lactic acid extract showed increased average lifespan and improved locomotor performance compared to those treated with methanolic extracts. In contrast, methanol-derived extracts significantly reduced survival and locomotor activity, likely due to residual solvent toxicity.

These findings demonstrate that solvent-solute interactions influence not only extraction yield but also in biological compatibility and functional performance*in vivo*. The integration of NADES and MAE enables the recovery of flavonoids in a stabilized and biologically compatible form, enhancing their antioxidant-related physiological effects. In particular , the choline chloride:lactic acid system emerges as a robust and sustainable alternative for the valorization of sugarcane bagasse.

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Strategies towards novel natural products from Brazilian cyanobacteria

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Palavras Chave:*cyanobacteria, secondary metabolites, metabolomics, genomics,cyanobacteria,secondary metabolites,metabolomics,genomics*

Highlights

Omics workflows streamline secondary metabolite discovery
Metabolomics revealed four new cyanobacterial peptides
Genome mining and BGCpri enables prioritization of NRPS, PKS, NRPS-PKS pathways

Resumo/Abstract

Cyanobacteria represent a prolific yet under investigated reservoir of natural products, providing valuable scaffolds for drug discovery. Broadening the diversity of biological sources and improving chemical screening strategies are essential for enhancing the discovery of bioactive molecules. In this work, we implemented metabolomic and genomic workflows to support the dereplication, prioritization, and discovery of secondary metabolites from Brazilian cyanobacterial strains. Within the metabolomics-driven strategy, a library of cyanobacterial fractions was generated and analyzed using UHPLC-HRMS-MS/MS alongside biological assays. Dereplication was achieved through the combined use of bioactivity networking, molecular networking, and SIRIUS, which enabled the identification of four novel bioactive peptides. In the genomics-based approach, we designed an automated prioritization tool, BGCpri, to identify and rank biosynthetic gene clusters (BGCs) in cyanobacterial genomes, focusing on NRPS, PKS, and hybrid NRPS–PKS pathways. The method was initially validated using the genome of*Moorena producens*JHB, a well-characterized cyanobacterial strain, and subsequently applied to publicly available genomes from Brazilian cyanobacteria. This analysis highlighted multiple BGCs with strong potential for further investigation. Overall, these findings emphasize the untapped potential of Brazilian cyanobacteria as sources of secondary metabolites and illustrate how combining metabolomic and genomic approaches can streamline natural product discovery.

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Structural and immunomodulatory properties of a (1→3),(1→6)-β-glucan from the edible Amazonian mushroom Gloeoporus thelephoroides

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Palavras Chave:*Amazonian rainforest, Wild edible mushroom, Gloeoporus thelephoroides, water-soluble beta-glucan, immunomodulatory properties,,Amazonian rainforest,Wild edible mushroom, Gloeoporus thelephoroides, water-soluble beta-glucan, immunomodulatory properties*

Highlights

*Gloeoporus thelephoroides*is a new Amazonian source of β-(1→3)(1→6)-glucan (*Gt*-BG1)*Gt*-BG1 shows potential for functional food and nutraceutical applications

Resumo/Abstract

β-Glucans from macrofungi are recognized as valuable bioactive compounds with immunomodulatory, antitumor, and antioxidant properties, driving demand for novel and sustainable sources. Despite an estimated 40,000 macrofungal species worldwide, fewer than 700 have been characterized for polysaccharide content, leaving Amazonian biodiversity particularly underexplored. This study aimed to extract, chemical composition and evaluate the immunomodulatory properties of β-glucan (*Gt*-BG1) from*Gloeoporus thelephoroides*, an edible wild mushroom from the Amazon biome. Structural analysis revealed that*Gt*-BG1 is composed of (1→3), (1→6)-β-linked glucose units, similar to lentinan from*Lentinula edodes*, but with a higher extraction yield, mainly from the gelatinous hymenophore.*Gt*-BG1 displayed a favorable biocompatibility profile, without affecting macrophage viability or proliferation. In contrast, it improved RAW 264.7 macrophages immune functions by increasing nitric oxide production, phagocytic activity, and changing their morphology. Although*Gt*-BG1 alone did not induce spontaneous cytokine release in bone marrow-derived macrophages (BMDMs) or dendritic cells (BMDCs) from C57BL/6 mice, it potentiated pro- and anti-inflammatory cytokine production following lipopolysaccharide (LPS) co-stimulation, particularly in macrophages, indicating an immuno-priming effect. These findings establish*G. thelephoroides*as a novel and promising source of bioactive β-glucans with potent immunomodulatory properties. The combination of high extraction yield, simple aqueous processing, and maintenance of cellular functional integrity during immune activation supports the potential application of*Gt*-BG1 in functional foods and nutraceutical development. This study highlights the biotechnological value of Amazonian macrofungi as sustainable sources of bioactive compounds and underscores the importance of biodiversity conservation for future bioprospecting initiatives.

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Study of the enaminone formation reaction from usnic acid and biological assays of the precursor and its derivatives

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Palavras Chave:*Usnic Acid; Enaminones; Semisynthesis; Antimicrobial Activity.*

Highlights

Usnic acid was modified to obtain new semisynthetic enaminone derivatives for biological evaluation.

Resumo/Abstract

Usnic acid, a secondary metabolite widely distributed in lichens belonging to the genera*Usnea*,*Ramalina*, and*Cladonia*, has been extensively investigated due to its remarkable biological potential[1]. Several studies report its broad spectrum of pharmacological activities, including antibacterial, antifungal, antiviral, anti-inflammatory, antiparasitic, and anticancer properties, characterizing it as a promising prototype molecule for the development of new drugs[2]. However, despite its relevant therapeutic potential, the clinical applicability of usnic acid is severely limited by its high hepatotoxicity, in addition to constraints related to solubility and bioavailability, factors that compromise its safety and efficacy[3]. In this context, the present study aims to obtain enaminones, derived from usnic acid, through semisynthetic strategies, seeking the generation of derivatives with potentially improved pharmacological profiles and reduced toxicity. The methodological approach is based on the structural modification of the C-2 carbon of usnic acid through reaction with different amines, conducted under reflux at 85 °C using absolute ethanol as solvent and triethylamine as an organic base. So far, one derivative has been obtained from*p*-anisidine, whose structure was confirmed by Nuclear Magnetic Resonance (NMR) spectroscopy, with a yield of 50.7%. Subsequent steps include the synthesis of new enaminone derivatives employing previously selected amines, followed by purification, structural characterization by ^{1}H and ^{13}C NMR, and biological evaluation of the compounds for leishmanicidal, trypanocidal, and antimicrobial activities.

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Study of the optimization of the antimicrobial activity of the essential oil and microemulsion of Pectis brevipedunculata (Asteraceae) in strawberries

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Palavras Chave:*Asteraceae, Food, Formulation, Fungi, Mesophilic aerobes.*

Highlights

-Oil and microemulsion of*P. brevipedunculata*increase strawberry shelf life.
-The microemulsion showed higher efficacy with lower MIC values.

Resumo/Abstract

Pectis brevipedunculata, a species of the Asteraceae family, popularly known as field rosemary, contains compounds, such as citral, that have antimicrobial, nematicidal, and larvicidal action. Despite being widely present in Brazil, the use of the plant is limited to the consumption of tea made from its aerial parts. This research aimed to obtain the essential oil (EO) from the aerial parts of*P. brevipedunculata*(EO-PB), develop a microemulsion (ME-PB) to incorporate the EO, apply it to strawberries, and investigate its antimicrobial potential. The EO extracted by hydrodistillation was chemically characterized by GC/MS and showed the following major components: α-pinene (56.47%), limonene (19.98%), neral (3.78%) and geranial (3.46%). Microemulsion (ME) analysis by GC/MS-Headspace and infrared confirmed the incorporation of the EO in the formulation. Physicochemical characterization showed that particle size, polydispersity index and zeta potential are in accordance with the literature. In terms of antimicrobial action, ME-PB showed inhibition halos above 50.00 mm for all bacteria tested (*Escherichia coli*,*Salmonella*spp.,*Listeria monocytogenes*,*Staphylococcus aureus*,*Bacillus cereus*and*Clostridium*spp.). In contrast, EO-PB showed smaller inhibition halos for all bacteria tested, except for*S. aureus*. ME-PB showed Minimum Inhibitory Concentration (MIC) values lower than those obtained with the action of the EO and demonstrated strong inhibition against all bacteria tested. It was observed that, when applied to strawberries, EO-PB and ME-PB proved effective against mesophilic aerobes and fungi, inhibiting the proliferation of microorganisms and prolonging the shelf life of strawberries. The results demonstrate the potential of*P. brevipedunculata*and that the incorporation of EO into the formulation optimized the bioavailability of bioactive principles and biological activity.

Agradecimentos/Acknowledgments

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Surviving the sludge: plant metabolic shifts triggered by the Fundão dam collapse

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Palavras Chave:*mining waste,abiotic stress,LC-MS/MS,Vernonanthura polyanthes,Piper aduncum*

Highlights

Plants activated species-specific biosynthetic pathways in response to the Fundão dam collapse. Peptide- and phenolic-centered axes were the principal detoxification mechanisms.

Resumo/Abstract

In November 2015, the sudden failure of the Fundão dam triggered a devastating environmental catastrophe, leaving widespread and lasting destruction across the state of Minas Gerais, Brazil. Over 40 million m^3 of mining waste containing various heavy metals spread across more than 650 kilometers of the Doce River basin, ultimately reaching the Atlantic Ocean and causing severe damage to terrestrial and aquatic ecosystems. While the immediate effects included the destruction of local habitats, certain endemic plant species demonstrated remarkable resilience by adjusting their metabolism to withstand extreme exposure to toxic mining waste. Herein, we employed an untargeted liquid chromatography-tandem mass spectrometry (LC-MS^n) metabolomics approach integrated with multivariate analysis and molecular networking to explore metabolic changes associated with the Fundão dam collapse in two traditional Brazilian medicinal plants,*Vernonanthura polyanthes*(Asteraceae) and*Piper aduncum*(Piperaceae). We found that, in response to exposure to toxic mining waste, plants triggered specific biosynthetic pathways that enhanced production of peptides, especially glutathione and lysine acetylated derivatives, for*V. polyanthes*, and phenylpropanoids, especially*O*-methylated*C*-glycosylated flavonoids, for*P. aduncum*. These changes are consistent with plant defense strategies, with*V. polyanthes*relying on a peptide-centered detoxification axis and*P. aduncum*on a phenolic-centered redox/defense axis, which reflecting the two principal detoxification pathways reported in plants under multi-metal stress conditions. Taken together, our results reveal metabolic shifts that support plant survival under extreme environmental disturbances, offering insights into ecological stabilization and metabolic adaptations underlying plant resilience.

Agradecimentos/Acknowledgments

The authors thank the support provided by FAPESP (#2020/02207, #2023/18392-4, #2024/02286-3, #2024/03447-0, and #2025/27006-6), INCT Nature #408549/2024-6), CNPq and CAPES.

Sustainable valorization of Couroupita guianensis as a source of indigo dye

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Palavras Chave:*Alkaloid; Natural dyes; Cannonball tree; Green extraction; Sustainability*

Highlights

• Indigo-rich extracts obtained from Couroupita guianensis

• Environmentally friendly process based on solvent-free extraction

• Valorization of problematic urban biomass in Rio de Janeiro

Resumo/Abstract

Indigo is a natural dye of major historical importance that has attracted renewed interest due to the growing demand for sustainable and renewable colorants. In parallel, the valorization of underutilized or problematic plant biomass in urban environments has emerged as a strategy aligned with the principles of green chemistry and the circular economy. In this context, the species Couroupita guianensis, widely used in urban landscaping in the city of Rio de Janeiro, stands out for generating large amounts of plant residues and is frequently associated with urban maintenance issues and inadequate biomass disposal.

This work describes a simplified and sustainable process for obtaining indigo-containing extracts from the fruit pulp of C. guianensis, focusing on mild extraction conditions without the use of organic solvents. The process consists of manual maceration of ripe fruit pulp, followed by solid–liquid extraction in an aqueous medium at a 1:2 (w/v) ratio under continuous agitation for 6–8 h. After filtration, the extract is centrifuged, the supernatant is discarded, and the precipitate is recovered and subjected to lyophilization. Parameters such as solvent composition, extraction time, and solid-to-solvent ratio will be systematically evaluated in order to maximize the indigo concentration in the crude extract while maintaining process simplicity and environmental compatibility.

The initially obtained extracts are being characterized by spectroscopic and chromatographic techniques, confirming the presence of indigo as the main chromophoric constituent. The proposed approach uses water exclusively as the extraction medium, eliminating the use of organic solvents. Thus, this study contributes to the valorization of problematic urban biomass in the municipality of Rio de Janeiro as a renewable source of natural dyes, adding value to plant residues and expanding the possibilities for the sustainable use of species widely distributed in urban areas.

Agradecimentos/Acknowledgments

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Synergistic Action of Volatile and Non-Volatile Metabolites from Bacillus velezensis PN2-45 in the Biocontrol of Fusarium spp.

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Palavras Chave:*Lipopeptides, surfactin, metabolomic analysis, antifungal activity.*

Highlights

Resumo/Abstract

Black pepper (*Piper nigrum*) is a globally significant spice, with Brazil being the second-largest producer. In Pará, production faces severe limitations due to endemic pathogens such as*Fusarium oxysporum*(FO) and*F. solani*f. sp.*piperis*(FSP), the causal agents of yellow wilt and root rot. Biocontrol through plant growth-promoting rhizobacteria represents a sustainable alternative to synthetic pesticides. This study performed a comprehensive metabolomic characterization of*Bacillus velezensis*PN2-45, elucidating its volatile and non-volatile secondary metabolites and their synergistic role in the biocontrol of*Fusarium*spp. Strain PN2-45 was isolated from healthy*P. nigrum*rhizospheres in Castanhal, Pará. Previous dual culture assays showed that PN2-45 inhibited FO and FSP mycelial growth by 72.9% and 63.1%, respectively. In sealed plate assays, bacterial volatile compounds inhibited FSP growth by 34.8%. GC-MS analysis identified dodecanal, n-decanal, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-3-buten-2-one, and 2-ethyl-hexanol as the main antifungal VOCs. The crude extract, obtained via liquid-liquid partition with ethyl acetate, was analyzed by LC-MS/MS. ESI(+) mass spectra enabled the manual annotation of seven major compounds: Bacillibactin (*m/z*883.2604 [M+H]+), Surfactin C12 (*m/z*994.6414 [M+H]+), Linear surfactin C15 (m/z 1054.6989 [M+H]+), Surfactin C13 (*m/z*1008.6570 [M+H]+), Surfactin C14 (*m/z*1022.6725 [M+H]+), Surfactin C15 (*m/z*1036.6875 [M+H]+), and Surfactin C16 (*m/z*1050.7034 [M+H]+). Other minor components, including fatty acids, amides, cytokinins, and diketopiperazines, were annotated using GNPS2 spectral libraries. The crude extract at 10 mg/mL inhibited FO by 39.93% and FSP by 56.32% by the well diffusion method. These findings suggest that the antagonism observed in dual culture assays is driven by the secretion of diffusible antimicrobial substances, a hypothesis corroborated by well diffusion assays and LC-MS/MS characterization.

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Target metabolic analysis of soybean sap (Glycine max (L.) Merril) with and without leaf wrinkling symptoms under field and greenhouse conditions

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Palavras Chave:*LC-MS,Biochemical fingerprinting,Isoflavones.,Isoflavones,Abiotic stress*

Highlights

Targeted metabolomics reveals distinct biochemical patterns in soybean sap.

Symptomatic plants show systematic changes in key metabolites.

Healthy plants present increased levels of isoflavones.

Resumo/Abstract

Leaf curling in soybean*(Glycine max (L.) Merrill)*is a disorder of unknown etiology characterized by leaf blade wrinkling and metabolic imbalance. This study aimed to perform targeted metabolic profiling of soybean sap to identify differentially expressed metabolites, particularly flavonoids and hormones, in plants with wrinkled symptoms (W) and healthy plants (H), collected from both field and greenhouse environments. Samples were obtained from the cultivar DM 66168IPRO. In field conditions, sap was extracted by stem centrifugation (5650 rpm, 20 min), whereas in greenhouse plants sap was collected via spontaneous exudation after horizontal stem cutting. Samples were lyophilized and analyzed by UPLC coupled to quadrupole mass spectrometry (Waters Acquity) with (PDA Photodiode Array) and QDA (Single Quadrupole Mass Detector) detectors using a C_{18} column. Metabolomic analysis revealed significant biochemical differences between symptomatic and healthy plants. Healthy plants exhibited higher concentrations of isoflavones, including daidzein, genistein, and their malonylated derivatives. These compounds are associated with redox homeostasis, chemical defense, and metal chelation, particularly of Mn^{2+}. The systematic reduction of these metabolites in symptomatic plants suggests impairment of defense pathways or metabolic reprogramming triggered by leaf curling–associated stress. The results indicate that metabolic profiling of the sap, often referred to as "plant blood," is a powerful tool for elucidating biochemical mechanisms underlying this disorder. This study provides a foundation for developing integrated management strategies focused on nutritional balance and microbial modulation to mitigate the impacts of leaf curling on soybean productivity.

Agradecimentos/Acknowledgments

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The IFA-BR network: connecting institutions and experts in Brazil to develop new green and chemical APIs inspired by Brazilian biodiversity.

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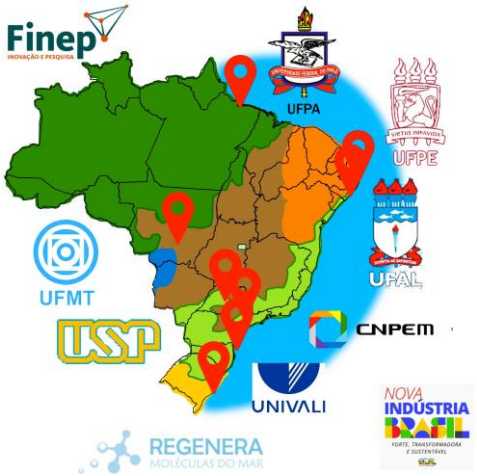
Palavras Chave:*Pharmaceutical innovation,Brazilian biodiversity,Active Pharmaceutical Ingredients (APIs),Health sovereignty*

Highlights

National network for pharmaceutical innovation based on biodiversity.
Advanced platform for the discovery of green and chemical APIs.
Development of APIs for priority diseases within the SUS.

Resumo/Abstract

Developing the national pharmaceutical innovation ecosystem is strategic for Brazil. Although molecules from biodiversity have historically been the main source of new active pharmaceutical ingredients (APIs) globally, and Brazil possesses the greatest biodiversity in the world, the country still has a high dependence on imports, with approximately 90% of APIs coming from abroad. In this sense, the IFA-BR network was consolidated as a joint effort of 7 Brazilian R&D institutions, funded by FINEP MCTI and co-financed by the company Regenera Moléculas do Mar. The project proposes the creation of a high-tech public-private network focused on radical pharmaceutical innovation from Brazilian biodiversity, to develop innovative APIs – both green and chemical – capable of meeting the priority demands of the Health Economic-Industrial Complex (CEIS) and the Unified Health System (SUS). The project is based on an advanced drug discovery platform, centered on omics, structural biology and data analysis, structured from a strategic bank of molecules from Brazilian biodiversity, in addition to resources in medicinal chemistry and pharmacology. Data mining techniques allow the mapping of the chemical space of different biomes, while predictive bioassays of clinical efficacy evaluate the pharmaceutical potential for diseases of great relevance to public health, such as cancer, inflammatory diseases and neglected diseases. As a case study, the project focuses on Psoriasis, an inflammatory disease with a high impact on the Brazilian Unified Health System (SUS), is being explored through an innovative therapeutic target based on molecules already at the TRL3 stage. Ultimately, the aim is to consolidate a functional national network for radical pharmaceutical innovation, a qualified bank of biodiversity molecules and APIs formulated for regulatory studies (TRL4+), establishing a solid foundation for the development of medicines 100% produced in Brazil.



IFA-BR network ilustration

The structural diversity of bacterial peptides has emerged as a privileged source of bioactive natural scaffolds for drug development

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Palavras Chave:*surugamidas – anticancer,depois termoactinamides,anticancer*

Highlights

• Natural peptide scaffolds for drug development

• Surugamide derivatives with selective anticancer activity

• Genomics-guided termoactinamide optimization against MDR bacteria

Resumo/Abstract

The structural diversity of bacterial peptides has emerged as a privileged source of bioactive natural scaffolds for drug development. Herein, we present consolidated results from our research program focused on the rational development of peptide derivatives with anticancer and antimicrobial activities, integrating advanced Nuclear Magnetic Resonance (NMR), molecular modeling, and genomics-guided discovery.

Among the investigated metabolites, surugamide derivatives have demonstrated significant anticancer potential. Structural modifications of the cyclic peptide scaffold resulted in improved biological profiles, including selective cytotoxic activity against tumor cell lines. Conformational analyses by 1D and 2D NMR, combined with in silico studies, revealed structural features consistent with interactions with molecular targets involved in tumor proliferation, including the transcription factor TBX2. Structure–activity relationship studies indicate that subtle modifications of the natural scaffold markedly influence biological response, reinforcing surugamides as versatile platforms for anticancer developmentOn the antimicrobial front, genomics-driven investigation of 65 bacterial strains enabled the identification of biosynthetic gene clusters associated with nonribosomal peptide production. This strategy guided the selection and optimization of termoactinamide and stigmurin derivatives, which exhibited relevant activity against multidrug-resistant Pseudomonas aeruginosa. NMR studies in solution and in biomimetic membrane systems suggest conformations compatible with membrane interaction, supporting a mechanism associated with bacterial membrane disruption.

These findings highlight bacterial peptides as strategic natural scaffolds for therapeutic innovation and demonstrate that the integration of genomics, rational chemical modification, and advanced NMR provides an efficient framework for accelerating the discovery of new bioactive candidates

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The authors acknowledge financial support from CNPq, and CAPES, as well as the international collaborations that contributed to the development of this research.

Three new labdane diterpenes from Campuloclinium purpurascens and their anti-Leishmania amazonensis activity

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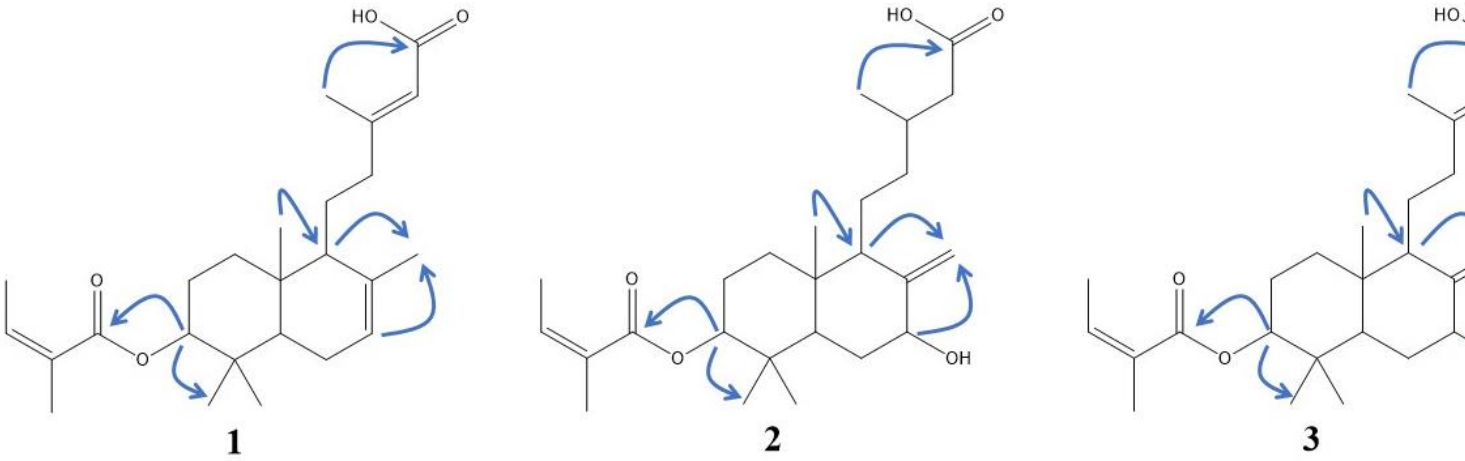
Palavras Chave:*Campos Gerais,Asteraceae,Eupatorium sensu lato.*

Highlights

First chemical investigation of*Campuloclinium purpurascens*. Isolation of three new labdane-type diterpenes. New labdanes present in the bioactive hexane fraction.

Resumo/Abstract

*Campuloclinium*is a genus segregated from*Eupatorium*comprising 12 species, of which only*C. macrocephalum*has been chemically investigated. Sesquiterpene lactones were previously described from a specimen collected in the Campos Gerais region of Paraná, Brazil.[1] Continuing our studies on*Eupatorium*sensu lato from this region, this work aimed to investigate the chemical composition of*Campuloclinium purpurascens*, a native Brazilian species. Chromatographic separations of hexane fraction on silica gel yielded three new labdanes-type diterpenes**(1-3)**. The structures were elucidated through comprehensive analysis of 1D and 2D NMR data. The ^{1}H NMR spectrum of**1**displayed signal for seven methyl groups, two olefinic methines, and one oxygenated methine. The ^{13}C NMR and HSQC data confirmed the presence of seven methyl groups and four methylene carbons, alongside two carbonyl signals at δC 170.9 (C-15) and δC 167.9 (C-1'). The structure was established from the HMBC spectrum by the correlations observed between H-3 (δH 4.41) with the carbons δC 167.9 (C-1') supported esterification at C-3 with a tigloyl group. The carboxylic acid moiety was assigned to C-15 based on correlations from H-16 (δH 1.93) to δC 170.9 (C-15) and δC 117.8 (C-14). Compounds**2**and**3**showed spectral profiles closely related to**1**, differing only in minor structural features**(Fig. 1)**. The crude extract and fractions were evaluated against*Leishmania amazonensis*and for cytotoxicity. The crude extract showed moderate cytotoxicity (CC_{50} = 92.7 µg/mL), whereas the hexane fraction exhibited significant activity against the amastigote form (IC_{50} = 5.95 µg/mL; SI = 7.26), despite higher cytotoxicity (CC_{50} = 43.2 µg/mL). Other fractions showed no relevant antiparasitic activity. These results constitute the first report on the chemistry of*C. purpurascens*, highlighting new labdane diterpenes present in the bioactive hexane fraction.



Compounds isolated from Campuloclinium purpurascens and key HMBC correlations.

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Turning waste into valuable secondary metabolites by bioconversion of banana peels-derived biomass with Aspergillus niger: Metabolomics insight.

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Palavras Chave:*food waste, banana peels, biomass, fermentation, Aspergillus niger, natural products.*

Highlights

- Food waste level including banana peels rises with urbanization
- Banana peels as biomass to grow*A. niger*
- Natural products produced from the bioconversion
- Annotation based on metabolomics approach

Resumo/Abstract

Santa Catarina is Brazil's fourth-largest banana producer, generating a significant amount of waste. Banana peel conversion into useful products is uncommon. However, it produces natural products that possess benefits for human health or can serve as biomass to produce fungi-derived metabolites. In general, the use of food waste for fungal cultivation not only produces valuable substances but also represents a cheap process when compared with conventional techniques that produce metabolites derived from micro organisms using purchased items. Therefore,*Aspergillus niger*was isolated from banana peels and then cultured on three distinct media composed of starch, banana peels (BP), and starch-enriched banana peels (BPS) for 14, 21, and 28 days at 28 °C. Their chemical profiles were established using liquid chromatography coupled to mass spectrometry data assisted by the GNPS database and MS-FINDER software. In BP media, 76 secondary metabolites were detected; among them, 66 were produced by the fungus. Twenty-seven compounds, such as nigragillin and pyranonigrin A, are*A. niger*chemomarkers, while other substances, except for the 13 unidentified, were previously found in other organisms. Among the 99 metabolites detected in BPS media, 22 were previously identified as*A. niger*-derived compounds. BPS media also yielded 26 unidentified compounds, while 12 annotated ones were also found in BP. The remaining metabolites were previously reported in other organisms. Principal component 1 of 44.8% and principal component 2 of 22.2% indicated that 21-day fermentation for BP medium and 28-day fermentation for BPS medium were the optimal conditions to produce secondary metabolites. Variable importance plots reveal nonadecan-2-amine (score >3) and an alkylaryl amine derivative (*m*/*z*304.3005) as the most concentrated compounds. The present results showed a cheap process to turn food residues and waste into valuable molecules.

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Uma nova γ-lactona dos galhos de Nectandra membranacea apresenta potencial anti-helmíntico in vitro e in vivo

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Palavras Chave:*Schistosomiasis, Schistosoma mansoni, Nectandra membranacea, - lactone.,Schistosomiasis,Schistosoma mansoni,Nectandra membranacea,γ-lactone*

Highlights

Bioassay-guided fractionation of hexane extract from*N. membranacea*branches led to the isolation of a new γ-lactone (membranaceolide) which displayed*in vitro*and*in vivo*activity against S. mansoni.

Resumo/Abstract

A esquistossomose é uma doença parasitária que afeta cerca de 250 milhões de pessoas, principalmente em países subdesenvolvidos. Visando identificar novo compostos com ação anti-helmíntica oriundos da biodiversidade florística brasileira, nesse trabalho, foi investigada a espécie vegetal*Nectandra membranacea*(Lauraceae). Inicialmente, foi obtida uma pequena quantidade de extrato hexânico dos galhos (100 mg) que se mostrou ativo,*in vitro*, frente ao*Schistosoma mansoni*. Após fracionamento cromatográfico em gel de Sephadex LH-20, foi obtido um composto puro (5 mg), que causou 100% de morte de vermes adultos a 100 µg/mL em 24 h e a 50 e 25 µg/mL em 48 h para machos e fêmeas, respectivamente. Os dados de RMN da substância isolada indicaram um sistema 2-alquil-3-hidróxi-4-metileno-γ-lactônico, confirmado por sinais característicos em δH 5,25 (H-3), 4,72 e 4,95 (H-5) e 7,08 (H-1'), além de sinais, dentre outros, em δC 166,8 (C-1), 157,8 (C-4) e 91,4 (C-5). O EMAR revelou os íons $[M+H]^+$ e $[M+Na]^+$ em*m/z*505,4629 e 527,4445, respectivamente, compatíveis com fórmula molecular $C_{33}H_{60}O_3$ para a substância isolada, indicando a presença de uma cadeia lateral com 28 carbonos. Assim, a estrutura foi determinada como mostrado na Figura 1, inédita na literatura e denominada membranaceolídeo. Visando a realização de experimentos*in vivo*, foi realizado novo fracionamento cromatográfico, de onde foram obtidos 50 mg do composto. Assim, a avaliação do potencial anti-helmíntico usando camundongos infectados, resultou em uma redução média de 57% da carga parasitária, inferior ao controle positivo praziquantel (90%) porém superior a outros produtos naturais tais como deidrodieugenol B (28%) e licarina A (50%). Assim, o estudo realizado com*N. membranacea*, uma espécie ainda desconhecida fitoquimicamente, resultou em uma nova γ-lactona com atividade anti-helmíntica*in vivo*, demonstrando o potencial da espécie como fonte de protótipos bioativos.

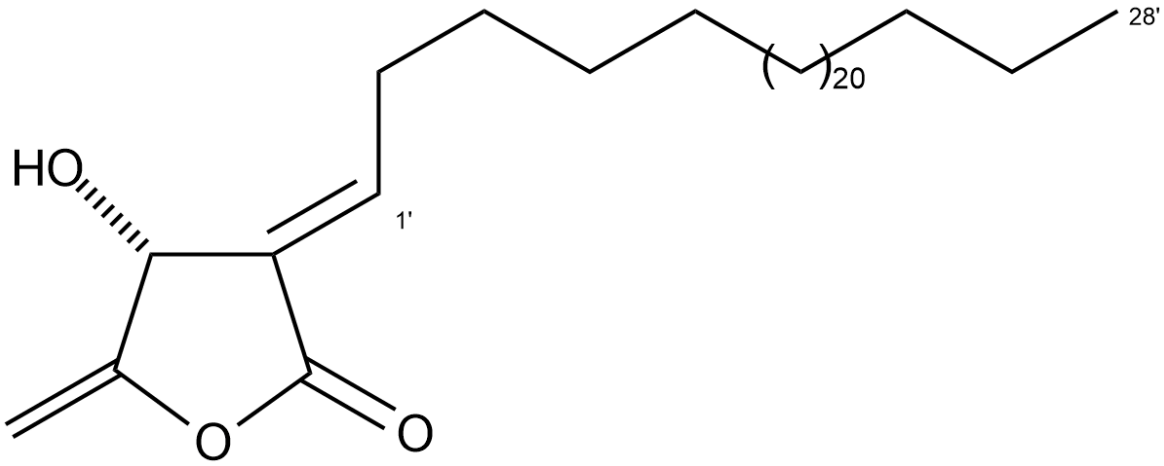


Figura 1: Formula estrutural da γ-lactona de N. membranacea com ação anti-S. mansoni.

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Untargeted metabolomics uncovers systemic root–shoot signaling underlying leaf wrinkling in soybean

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Palavras Chave:*Untargeted metabolomics,LC-MS,Leaf curling disorder,Root–shoot signaling,Brazilian agricultural innovation*

Highlights

- Leaf curling was associated with systemic root–shoot metabolic reprogramming;
- Root metabolomic shifts preceded and shaped leaf metabolic responses.

Resumo/Abstract

Soybean (*Glycine max*(L.) Merr.) is a strategic crop whose productivity can be compromised by leaf curling, a complex disorder linked to soil acidity, calcium deficiency, and manganese and boron toxicity. Although plausible, its cause(s) remain unclear and may involve interacting mechanisms. Despite its relevance, the molecular basis of this phenomenon remains poorly understood, especially from metabolomics. This study aimed to characterize the metabolomic profiles of soybean leaves and roots affected by leaf curling using high-resolution mass spectrometry, with a focus on systemic signaling and reprogramming of secondary metabolism. Multivariate analyses revealed clear metabolic discrimination between symptomatic and asymptomatic plants, as well as between roots and leaves. Unsupervised PCA of leaf and root extracts acquired in positive and negative ionization modes showed consistent clustering by tissue and disease status, while OPLS-DA confirmed this separation and identified key discriminant metabolites underlying coordinated root–shoot responses. In symptomatic plants, high-VIP (> 1.00) metabolites were predominantly associated with isoflavonoid metabolism, triterpenoid saponins, lipid-derived signaling molecules, and nematode-related ascarosides. Leaves were characterized by the accumulation of genistein and soyasaponins, indicating activation of the phenylpropanoid and flavonoid pathways, as well as oxylipins linked to jasmonate-mediated stress signaling. Notably, the detection of multiple ascaroside homologues supports systemic root–shoot communication in response to belowground biotic stress. In roots, the metabolic signature was dominated by triterpenoid saponins and isoflavonoids, including daidzin and pratol, reflecting early stress perception under acidic soil conditions. This study provides the first field-based metabolomic evidence of coordinated root–shoot reprogramming associated with leaf curling in soybean under Brazilian agricultural conditions.

Agradecimentos/Acknowledgments

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Unveiling the absolute configuration of Ruehssiosides A–R, pregnane glycosides isolated from the roots of Ruehssia caatingae.

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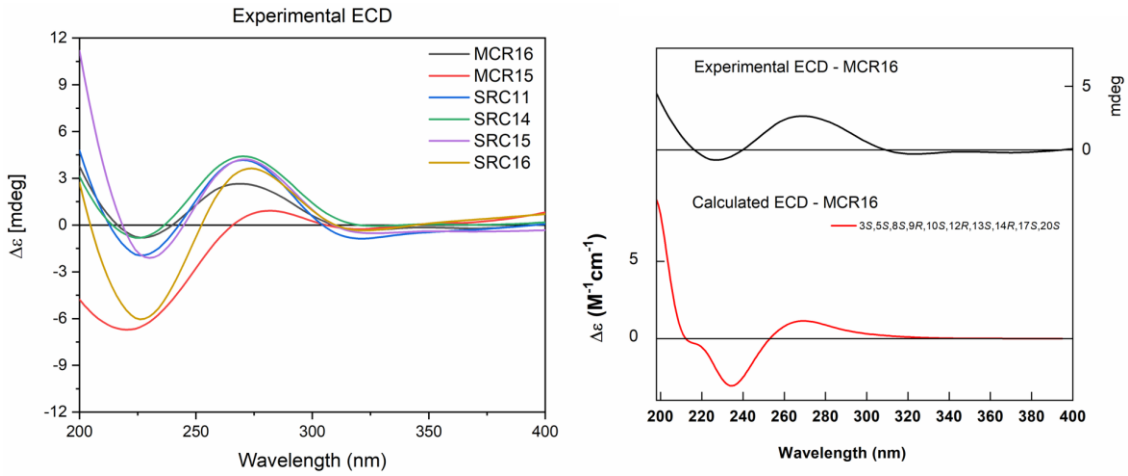
Palavras Chave:*Natural Products,Electronic Circular Dichroism,Molecular Modeling,TD-DFT,Stereochemistry*

Highlights

In this work, the absolute configuration of the A–R Ruehssiosides is unequivocally determined by means of electron circular dichroism spectroscopy, along with quantum chemical simulations.

Resumo/Abstract

Since the suggestion of Van't Hoff and Le Bel that individual molecules could present a tridimensional structure would lead to dissymmetry, determine the exact spatial orientation of the atoms, in other words, the absolute configuration (AC), became one of the most important and challenging tasks in the field of molecular stereochemistry. Since enantiomers can present different biological properties, AC elucidation of secondary metabolites is a fundamental step in drugs discovery. In this work, our focus is determining the AC of Eighteen New Pregnane Glycosides, called Ruehssiosides A–R, from the roots of Ruehssia caatingae. This plant is widely found in semi-arid region of northeastern Brazil, specially in Caatinga. These compounds were isolated by Professor Josean Tavares Fechine's workgroup (UFPB) and his relative configurations were established previously mainly through NMR 1D and 2D spectroscopy. The ACs were determined by the comparison of Electronic Circular Dichroism (DCE) spectra of the isolated compounds with their corresponding simulated spectra. The experimental ECD spectra of isolated samples from Ruehssia caatingae (1mg/mL) were obtained in acetonitrile, in a JASCO J-1100 spectrometer (JASCO Tokyo Japan). The corresponding simulated spectra were obtained from time-dependent formalism of Density Functional Theory (TDDFT), at CAM-B3LYP/TZVP//B3LYP/6-31G(d) level. To considered the solvent effects, the polarizable continuum method (PCM) was applied. All the quantum mechanical calculations were executed in Gaussian 09 software.



Electronic Circular Dichroism spectra of isolated samples from Ruehssia caatingae

Agradecimentos/Acknowledgments

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Unveiling the chemical profile and biological activity of Phyllosticta sp.: insights into endophytic-phytopathogenic interactions in citrus.

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Palavras Chave:*Citrus black spot,Phyllosticta,Endophytic Fungi,Citriculture*

Highlights

Secondary metabolites in Phyllosticta are associated with ecologial roles. Endophytic Phyllosticta sp. extracts show antifungal activity against P. citricarpa. LC-MS revealed diverse bioactives classes.

Resumo/Abstract

Citrus Black Spot (CBS), caused by*Phyllosticta*citricarpa, is one of the most severe phytosanitary diseases affecting citrus crops in Brazil, leading to virulent lesions, premature fruit drop, and significant economic losses. The widespread use of synthetic fungicides highlights the urgent need for sustainable control strategies. In this context, endophytic fungi of the genus*Phyllosticta*have emerged as promising sources of bioactive specialized metabolites (SMs) for biocontrol. However, the chemical basis underlying interactions between endophytic-phytopathogenic*Phyllosticta*species remains poorly understood. In this study, the inhibitory effects of*Phyllosticta*sp. against*P. citricarpa*were investigated through integrated chemical and biological analyses. Fractions from the crude extract of the endophyte were generated by chromatographic separation and evaluated for antifungal activity. These fractions were solubilized in DMSO:H_2O(5:95) and tested in 6-well microplates using potato dextrose agar. Each well was inoculated with 2 µL of a spore suspension 10^6 spores·mL^{-1} of*P. citricarpa*. Assays were conducted at 300 ppm in triplicate, with imazalil as a positive control. Several fractions significantly inhibited*P. citricarpa*growth, indicating the presence of potent bioactive metabolites. Chemical profiling was performed via LC-HRMS (Orbitrap, positive mode), with data processed using MZmine for feature-based molecular networking and SIRIUS for annotation. Detected compound classes included 2-pyrone derivatives, guignardones, coumarins, macrolides, peptides, and alkaloids. To explore biosynthetic potential, publicly available genomes were analyzed using antiSMASH and BiG-SCAPE, revealing shared biosynthetic gene clusters (BGCs) related to PKS, PKS–NRPS, RiPPs, and terpene pathways. Overall, this study highlights the chemical relevance of endophytic–phytopathogenic interactions and contributes to the discovery of SMs with aplications in CBS management.

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Use of agro-industrial waste as biocatalysts for the transformation of Emerging Organic Pollutants

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Palavras Chave:*Emerging organic pollutants; biodegradation; agro-industrial waste; winemaking waste, brewery waste.,Emerging organic pollutants,biodegradation,agro-industrial waste,winery waste,brewery waste*

Highlights

Organic pollutants consist a problem; lack of regulation is a public health problem; Agro-industrial waste is an environmentally, and sustainable alternative for the degradation of organic compounds.

Resumo/Abstract

Emerging Organic Pollutants, are substances commonly found in a wide range of marketed products, such as antibiotic drugs, analgesics, steroidal or non-steroidal anti-inflammatory drugs, for psychiatric use and contraceptives, as well as veterinary materials, food packaging and pesticides. They have been a topic of significant interest within analytical and biotransformation chemistry.

This work deals with the use of winery and brewery waste, important industries within the regional economy. In this scenario, the production of the brewing industry reveals itself as a potential source of raw material to Biorefineries, providing them with biological materials resulting from the fermentation and malting process, serving as a source of biocatalysts and biodigestion materials. The state of RS is the largest producer of grapes and wines in the country, contemplating a total area of 47,000 hectares and 539 wineries located in the state. According to EMATER data, the production estimate for the 2023/2024 harvest is to reach a production of 719,000 tons of grapes, corresponding to more than 1% of the state PIB.

The choice of these two types of waste is due to the amount of integral enzymes present in the waste (and consequent reactivity of both. 10 g of the different residues were used, a specific mass of selected commercial medicines (ibuprofen, prednisone, and acetylsalicylic acid) were added and left under agitation in a closed balloon for 3 days under agitation, then the sample is filtered, liquid-liquid extraction with ethyl acetate and evaporated route, later the sample is analyzed in GC/MS to determine the reaction products where the reduction of carbonyl compounds was observed, thus demonstrating the presence of reductase-type enzymes, and in case for acetylsalicylic acid with a brewery waste The formation of compounds from transesterification were detected and that this type of agro-industrial waste can act as a source of enzymatic material for reactions.

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Use of TD-NMR for the Evaluation of the Quality of Organic Maize Seeds Coated with Curcuma longa, Schinus terebinthifolius, and Dysphania ambrosioides

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Palavras Chave:*Organic corn,TD-NMR,Vegetable oils*

Highlights

Time domain NMR was applied as a rapid, non destructive tool to assess organic corn seed quality.

TD-NMR replaces traditional destructive methods, avoiding solvents and reducing analysis time and cost.

Resumo/Abstract

This study evaluated the application of Time-Domain Nuclear Magnetic Resonance (TD-NMR) as a tool for analyzing the quality of organic maize seeds. Traditionally, seed structural integrity is determined by classical methods based on drying, grinding, and extraction with organic solvents, which, although effective, are destructive, time-consuming, and dependent on the use of chemical reagents. In this context, TD-NMR offers relevant advantages, such as rapid analysis, non-destructive nature, absence of solvents, and low operational cost, establishing itself as a promising technique for applications aimed at conservation and sustainable agricultural production. Organic maize seeds were subjected to two treatment methods (direct contact and fumigation) with three distinct plant oils (Curcuma longa, Schinus terebinthifolius, and Dysphania ambrosioides) and stored for 13 months in two different environments (cold chamber and uncontrolled environment). Seed quality was evaluated through transverse relaxation parameters (T_2), using an inter-pulse time between 90° and 180° pulses of 0.05 ms. The results indicated that lower T_2 values were associated with reduced mobility of hydrogen nuclei in water molecules, suggesting better preservation of the biological structure of the seeds. Treatments with oils of Curcuma longa, Dysphania ambrosioides, and especially their combination, applied by fumigation and stored in a cold chamber, showed some of the lowest and most consistent T_2 values. These findings are consistent with literature data, such as those reported by Nascimento (2025), who observed a biostimulant effect of Curcuma longa on maize seeds, reflected in an increased germination rate, reinforcing the robustness of TD-NMR as a tool for monitoring seed quality.

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Virola officinalis: diversidade molecular de uma planta com usos etnobotânicos entre os Pataxós

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Palavras Chave:*Virola officinalis,Fitoquímica*

Highlights

Characterization of the molecular diversity of Virola officinalis of different parts of the plant through spectroscopic and spectrometric analyses

Resumo/Abstract

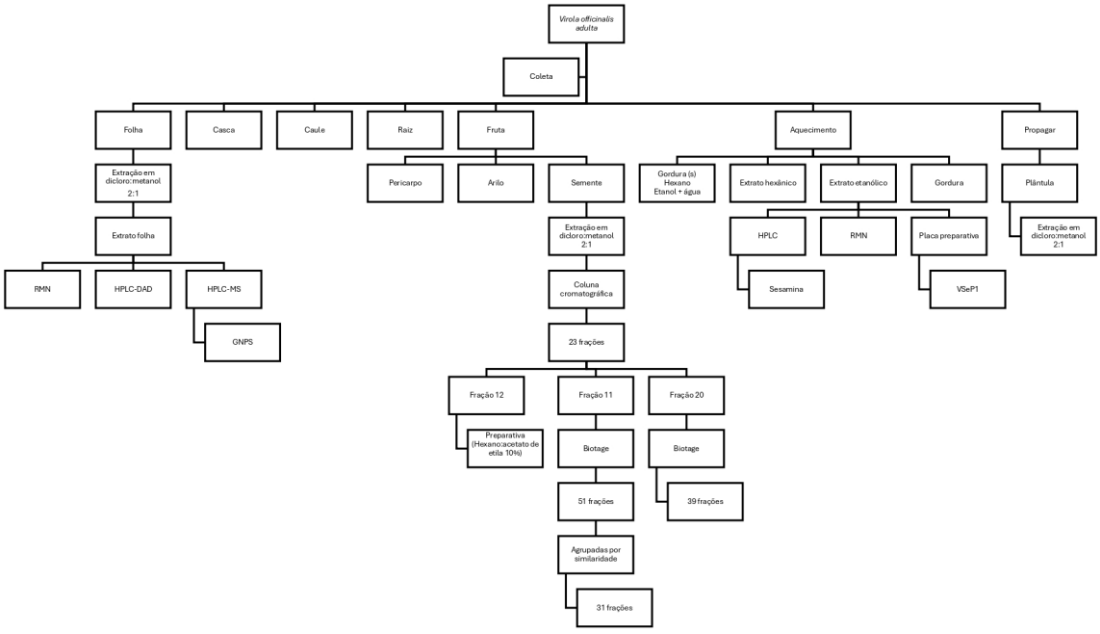
O gênero*Virola*pertence à família Myristicaceae e compreende cerca de 70 espécies [1]. A espécie*Virola officinalis*é endêmica da Mata Atlântica e possui usos etnofarmacológicos entre os Pataxó. O óleo obtido das sementes é empregado no tratamento de infecções fúngicas cutâneas [2]. Porém, não há relatos de estudos fitoquímicos. Assim, o objetivo do projeto é caracterizar a diversidade molecular das diferentes partes da planta (frutos, caules, folhas) e plântulas.

Foram obtidos extratos da planta*V. officinalis*coletada em Arraial d'Ajuda (BA). O material vegetal foi seco, triturado e macerado em diclorometano:metanol (2:1) e analisado por HPLC-MS, revelando similaridade química entre os extratos, por redes moleculares no GNPS.

O extrato da semente foi submetido à remoção de triglicerídeos por cristalização em etanol a quente seguido de extração com hexano. A análise do espectro de RMN de ^{1}H da fração hexânica indicou um predomínio de triglicerídeos, mas também compostos aromáticos com grupamentos metilenodioxifenílicos, metoxílicos e enonas (~δ 18 ppm). Na fração etanólica observaram-se sinais característicos de lignanas furofurânicas, incluindo kobusina e sesamina, confirmada pelo uso de padrões em HPLC. A cromatografia líquida sob vácuo permitiu o fracionamento do extrato em 23 frações. Após análises de RMN ^{1}H, a fração 11 foi submetida a placa preparativa, e as frações 12 e 20, em Biotage. A análise por RMN ^{1}H revelou a presença de lignanas, triglicerídeos e enonas (fração 11). A partir da fração 20, obteve-se, de forma quase pura, a lignana kobusina [2]. Desta forma, o estudo amplia o conhecimento fitoquímico acerca da*V. officinalis*. Posteriormente, os extratos e frações serão testados quanto a atividade antifúngica.

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[2] Rodrigues, W. A. (2010). Flora of Bahia: Myristicaceae. SITIENTIBUS série Ciências Biológicas, 10(1), 138–146



Fluxograma do procedimento experimental realizado

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