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Caderno de Resumos

Anais da 43ª Reunião Anual Virtual da SBQ

https://proceedings.science/rasbq-2020

Galoá

Alimentos e Bebidas - BEA

Addition of flaxseed flour as a substitute for eggs in cupcakes: fatty acid profile

https://proceedings.science/p/122925

Tatiane Bertoldo [1]; Daneysa Lahis Kalschne [2]; Diogo Salvati [1]; Alex Sanches Torquato [1]; Aloisio Henrique Pereira de Souza [3]; Angela Claudia Rodrigues [1]

[1] Universidade Tecnológica Federal do Paraná; [2] Universidade Estadual de Londrina; [3] Instituto Federal de Mato Grosso do Sul

Elaboration of cupcakes without eggs, containing PF and FF flour. Formulations with a high content of α-linolenic acid (n-3). Acceptable content of saturated FAs.

ANÁLISE DO PERFIL DE QUÍMICO DE SUCO DE UVA PRODUZIDO NA REGIÃO DE MINAS GERAIS POR IONIZAÇÃO AMBIENTE PS/MS NO MODO NEGATIVO

https://proceedings.science/p/119924

Henrique de Oliveira Prata Mendonça [1]; Miriã Cristina Pereira Fagundes [2]; Mariana A. P. Barbosa [3]; Ana Luiza Coeli Cruz Ramos [4]; Rodinei Augusti [5]; José Carlos Moraes Rufini [6]; Luisa del Carmen Barrett Reina [7]; Yesenia Mendoza García [8]; Altamir Fernandes de Oliveira [9]; Julio Onésio Ferreira Melo [6]

[1] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [2] Universidade Estadual de Santa Cruz; [3] Universidade Federal de São João del-Rei - Campus Alto Paraopeba; [4] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [5] Universidade Federal de Minas Gerais; [6] Universidade Federal de São João Del Rei; [7] Universidade Federal de Mato Grosso; [8] Universidade Federal de Alagoas ; [9] Universidade Federal dos Vales do Jequitinhonha e Mucuri

The ambient ionization technique allowed the identification of antioxidant and bioactive compounds present in grape juice, demonstrating the commercial potential of the study region.

ANÁLISE DO PERFIL QUÍMICO DE SUCO DE UVA PRODUZIDO NO CENTRO-OESTE POR IONIZAÇÃO AMBIENTE PS/MS NO MODO NEGATIVO

https://proceedings.science/p/120747

Ariele Oliveira Franco [1]; Henrique de Oliveira Prata Mendonça [2]; Afonso Henrique De Oliveira Júnior [3]; Priscilla Nascimento [4]; Yuri Gomes Figueiredo [5]; Mércia Aurélia Gonçalves Leite [6]; Francielly da Encarnação Amorim [6]; Miriã Cristina Pereira Fagundes [7]; Ana Luiza Coeli Cruz Ramos [8]; Rodinei Augusti [9]; Luisa del Carmen Barrett Reina [6]; Yesenia Mendoza García [10]; Julio Onésio Ferreira Melo [1]

[1] Universidade Federal de São João Del Rei; [2] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [3] Universidade Federal de São João del-Rei; [4] Universidade Federal de São João del-Rei - Campus Alto Paraopeba; [5] Universidade Federal de São João del Rei (campus Sete Lagoas); [6] Universidade Federal de Mato Grosso; [7] Universidade Estadual de Santa Cruz; [8] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [9] Universidade Federal de Minas Gerais; [10] Universidade Federal de Alagoas

Analysis of Grape Juice Chemical Profile Produced in Central West With PS/MS Environment Proionization in Negative Mode. The PS-MS technique identified compounds with antioxidant and bioactive characteristics beneficial to health in the samples of grape juice.

ANÁLISE DO PERFIL QUÍMICO DE SUCO DE UVA PRODUZIDO NO CENTRO-OESTE POR IONIZAÇÃO AMBIENTE PS/MS NO MODO POSITIVO

https://proceedings.science/p/119892

Henrique de Oliveira Prata Mendonça [1]; Yuri Gomes Figueiredo [2]; Mércia Aurélia Gonçalves Leite [3]; Paula Becker Pertuzatti Konda [3]; Ana Luiza Coeli Cruz Ramos [4]; Rodinei Augusti [5]; Luisa del Carmen Barrett Reina [3]; Yesenia Mendoza García [6]; Miriã Cristina Pereira Fagundes [7]; Altamir Fernandes de Oliveira [8]; Julio Onésio Ferreira Melo [9]

[1] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [2] Universidade Federal de São João del Rei (campus Sete Lagoas); [3] Universidade Federal de Mato Grosso; [4] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [5] Universidade Federal de Minas Gerais; [6] Universidade Federal de Alagoas ; [7] Universidade Estadual de Santa Cruz; [8] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [9] Universidade Federal de São João Del Rei

Analysis of Grape Juice Chemical Profile Produced in Central West with PS/MS Environment Ionization in Positive Mode. The PS-MS technique identified compounds with antioxidant and bioactive characteristics in grape juice.

Análise físico-química e bromatológica dos açaís (Euterpe sp) comercializados no Médio Solimões

https://proceedings.science/p/120766

Klenicy Kazumy de Lima Yamaguchi [1]; Leilson Nascimento Oliveira [1]; Eldrinei Gomes Peres [1]
[1] Universidade Federal do Amazonas

Assai marketing is little described;
Two species can be found in Amazon region;
There are few comparative studies on açaí sold in different countryside in Amazonas

Analysis and differentiation of craft worts through the direct determination of amino acids by capillary electrophoresis and multivariate analysis

https://proceedings.science/p/120742

Rafaella Silva Aredes [1]; Fernando Peixoto [2]; Leandro Alcoforado Sphaier [1]; Flávia Ferreira de Carvalho Marques [1]
[1] Universidade Federal Fluminense; [2] Instituto Militar de Engenharia

A new tool for control, identity and beer quality assurance, was developed through amino acids in beer and beer worts analysis by electrophoresis and Principal Component Analysis.

Analysis of tabletop sweeteners by liquid chromatography coupled with mass spectrometry: identifying irregularities in commercial products

https://proceedings.science/p/119677

Igor Forattini Prates Carvalhais Noronha [1]; Clésia Cristina Nascentes [1]; Maria Beatriz de Abreu Glória [1]
[1] Universidade Federal de Minas Gerais

The use of high intensity sweeteners (HIS) has increased nowadays, due to worries about the consequences of high sugar consumption and weight gain. The active principles of sweeteners are molecules with higher sweetening power than sucrose and a small (or none) caloric contribution. As so, this study aimed to determine some synthetic HIS [saccharin (SAC), cyclamate (CYC), aspartame (ASP), acesulfame-K (ACS) and sucralose (SUC)], and two of the main compounds extracted from *Stevia rebaudiana* [stevioside (STV) and rebaudioside A (RBD)], used as a natural sweetener, in commercial tabletop sweeteners (n=50).The obtained results were then compared with the information on the product label. Before analysis, solid samples were homogenized, 10,0 mg were weighted in polyethylene tubes and solubilized in 50,0 mL of ultrapure water. For liquid samples, an aliquot of 10,0 µL (approximately 10,0 mg) was transferred to polyethylene tubes and diluted to 50,0 mL. A second dilution was performed to match the concentration of the samples to the calibration curve. Finally, the samples were analyzed by liquid chromatography coupled with sequential mass spectrometry (LC-MS/MS), using a validated method. Among analyzed samples, 7 (14%) were labeled as natural product, but 3 (43%) of them presented synthetic HIS in their composition. In products which report that they're a mixture of synthetic and natural sweeteners (n=3, 6% of the samples), the amount of natural sweeteners is much lesser than the synthetic ones. In addition, 8 samples (16%) had informed on their label the content of each HIS in their composition, which has allowed a comparation between the obtained value and the informed one by a t-test. Some irregularities were found, indicating that improvements in quality control of these products are needed.

Avaliação do perfil químico da farinha extrusada de sorgo do genótipo BRS 305 utilizando a espectrometria de massas com ionização por paper spray

https://proceedings.science/p/120744

Vinícius Tadeu da Veiga Correia [1]; Danielle Fatima D'Angelis [2]; Maria Clara Coutinho Macedo [1]; Viviane Dias Medeiros Silva [1]; Ana Luiza Coeli Cruz Ramos [3]; Ana Paula Xavier Mariano [1]; Rodinei Augusti [1]; Valéria Queiroz; Andreza Angélica Ferreira [1]; Camila Argenta Fante [1]; Julio Onésio Ferreira Melo [4]
[1] Universidade Federal de Minas Gerais; [2] Universidade Federal do Oeste do Pará; [3] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [4] Universidade Federal de São João Del Rei

With the analyzes, the chemical composition of extruded sorghum flour was obtained, where compounds with antioxidant and bioactive properties were identified.

Avaliação térmica de edulcorantes comerciais

https://proceedings.science/p/119699

Millena Lima Almeida [1]; Aline Maria Viana de Souza [1]; Tatiani da Luz Silva [2]
[1] Universidade do Estado do Pará; [2] Universidade Federal do Sul e Sudeste do Pará

A concern regarding the use of sweeteners is in relation to their thermal stability, as several principles active substances currently replace ordinary sugar used in vast majority for therapeutic purposes, for those who have diabetes problems or even weight loss, for presenting restrictions on use when the product suffers some temperature change, a fact that occurs when they are added to hot drinks and are used in the preparation of food that will go through the frying or cooking process. In the literature, there are few information regarding the thermal behavior of these sweeteners and much unproven information scientifically published on the internet. Thus, this work aims to analyze the thermal behavior of four commercial samples of sweeteners purchased from the same manufacturer in the same establishment commercial. Each sample has a different active ingredient and some have restrictions on the use in hot foods. The analyzes were performed in the thermal analysis laboratory of the Federal University of South and Southeast of Pará (UNIFESSPA).

Bioaccessibility of Cd, Cu, Fe and Zn in basil samples (Ocimum Basilicum L. grecco a palla) after Cd intoxication

https://proceedings.science/p/120304

Letícia Malta Costa [1]; Sofia Martins [1]; Vania de Lourdes das Graças Teles [1]; Giselle Sousa [1]
[1] UFMG

The bioaccessibility, defined as the amount of metal that is converted to soluble forms in the gastrointestinal conditions can be evaluated by sequential analysis with artificial gastric and intestinal juices. The analysis of the soluble fractions is widely used to evaluate bioaccessibility of minerals and trace elements from different food products [1]. In this study, the bioaccessibility of Cd, Cu, Fe and Zn was accessed in basil samples after Cd intoxication. The seeds were germinated in Germitest paper until the roots length ~ 0.5 cm. Afterwards, radicle were grown in hydroponic solution, using 5% v v-1 Hoagland solution. The cuttings were exposed to Cd2+ [as Cd(NO3)2.4H2O] to varying concentrations (0, 1.5 and 3.0 mol L-1). Hoagland solution were replaced each 3 days and after 15 days the plants were transferred to vermiculite pots and kept for another 15 days, to increase the quantity of leaves. In vitro gastrointestinal [2] were applied in fresh and lyophilized samples. After, 1 mL of the digested sample were sonicated in a cup horn ultrasound, adding 100 µL HNO3 and 500 µL H2O2. Final volume was completed to 2 mL. Total concentration was achieved after microwave (MW) acid digestion. Limits of detection and quantification after MW digestion for Cd, Cu, Fe and Zn were 0.07 and 0.23, 0.6 and 1.99, 10.7 and 35.3, 8.5 and 27.9 g L-1, respectively. Total concentrations and bioaccessibility values presented in Table 1 were obtained after quantification by ICP-MS.

Caracterização físico-química da farinha obtida a partir de uma Planta Alimentícia Não-convencional: Dioscorea bulbifera Linn

https://proceedings.science/p/120752

Ani Caroline Weber [1]; Bruna Costa [1]; Gabriela Kuhn [1]; Daniel Weber [1]; Ana Giacomin [1]; Lucélia Hoehne [1]; Eduardo Miranda Ethur [1]
[1] Universidade do Vale do Taquari

Physico-chemical characterization of flour obtained from air potato.
Knowledge of unconventional food plants.
Flour with characteristics beneficial to health.

Centesimal Composition of Nutritional Bar Prepared with Quercetin

https://proceedings.science/p/119956

Halliny Ruela [1]; Erika B. Fonseca [2]; Marina G. Oliveira [2]; Norma da Rocha [2]; Jaqueline Peixoto [3]; Christian da Silva [3]; Anna Paola Trindade Rocha Pierucci [3]

[1] Hospital Naval Marcílio Dias / Instituto de Pesquisas Biomédicas / Laboratório de Bioanálises; [2] Laboratório Farmacêutico da Marinha / Departamento de Pesquisas em Ciências Farmacêuticas; [3] Universidade Federal do Rio de Janeiro / Instituto de Nutrição Josué de Castro, Laboratório de Desenvolvimento de Alimentos para Fins Especiais e Educacionais

This work shows the centesimal composition and quercetin content of a nutritional bar. It's complies with the legislation, having potential for registration as a functional food.

CHARACTERIZATION OF HONEY FROM MELIPONINAE AND APIS MELLIFERA BEES

https://proceedings.science/p/120204

Ednei Gilberto Primel [1]; Jean Lucas de Oliveira Arias [2]; Sergiane Caldas Barbosa [1]; Andrea Carolina Begambre Berrio [1]; Luanne Ramos Lima [1]; Lucas Cavagnoli Marcolin [1]

[1] Universidade Federal do Rio Grande-FURG; [2] Universidade Federal do Rio Grande - FURG

CHARACTERIZATION OF HONEY FROM MELIPONINAE AND APIS MELLIFERABEES Ednei G. Primel (PQ)1,Jean L.O. Arias (TC)1,Sergiane C. Barbosa (PQ)1, Andrea Begambre (PG)1, Luanne R. Lima (IC)1, Lucas C. Marcolin (PG) 1* eprimelfurg@gmail.com; lucas--marcolin@hotmail.com 1Federal University of Rio Grande, School of Chemistry and Food. Avenida Itália, km 08, Carreiros, Rio Grande, RS, Brazil Key words: Food, Honey, Legislation, Quality, Identity. Honeycanbeproducedbyseveralspeciesofbees, includingbeesfromtheMeliponinaetribe, known as nativebeesthat do nothave a stingers, andfromthetribeofAfricanizedbeeswherethereis a predominanceoftheApismelliferaspeciesthathavestingers. The honeycompositionofthesespeciescanvary, anddependson some factorssuch as the floral andgeographicsource, climateandseason, processingandstorage (BONTÉ; DESMOULIÈRE, 2013, BRASIL, 2000). The presentworkaimstocharacterizethemitesoffivespeciesofstinglessbees (Meliponinae) andwithstingers (Apismellifera) fromthreemunicipalities in Rio Grande do Sul state. The parametersdeterminedwere pH, electricalconductivity, freeacidity, humidity, ashes, 5-hydroxymethylfurfural (HMF)andsugarsfructose, glucose andsucrose Table 1 presentstheresultsoftheidentityandqualityparametersofthehoney samples fromthreedifferentmunicipalities in thestateof RS. Table 1 - Physico-chemicalcharacteristicsofhoney samples frombeesofthespeciesMeliponinaeandApismellifera Species City pH Conductivity (mS/cm) Freeacidity (mEq/kg) Humidity (% m/m) Ashes (% m/m) HMF (% m/m) F + G (%) Sucrose (% m/m) Apis m RG 4.0±0.0d 0.38±0.0d 23.2±0.5c 17.2±0.0e 0.09±0.0b 14.5±0.3a 62.9±3.4ab 12.1±0.6c Tubuna GR 4.3±0.0bc 1.1±0.0a 67.4±2.7a 27.8±0.4b 0.49±0.1a 0.0±0.0e 53.9±1.1cd 12.4±0.1c Mandaçaia GR 4.2±0.0cd 0.19±0.0ef 17.7±2.4de 28.2±0.7b 0.11±0.0b 1.9±0.2c 58.3±5.1cd 7.6±0.7ef Jataí GR 4.3±0.1bc 0.78±0.0c 66.7±2.3a 26.0±0.9c 0.32±0.2ab 3.9±0.9b 55.4±0.5c 15.5±0.3b Apis m GR 4.3±0.0bc 0.91±0.0b 28.1±0.5b 20.4±0.7d 0.58±0.1a 0.0±0.0e 62.5±1.5ab 7.8±0.4e Guaraipo IL 4.2±0.0bc 0.14±0.0g 11.2±0.1e 32.3±0.0a 0.07±0.0b 1.0±0.0d 54.3±0.5c 8.6±0.2e Manduri IL 4.3±0.0bc 0.15±0.0gf 13.1±0.8e 31.7±0.5a 0.08±0.0b 0.5±0.2de 53.3±1.3cd 10.4±0.4d Tubuna IL 4.4±0.0b 0.20±0.0e 14.3±0.3ef 28.9±0.2b 0.12±0.0b 0.8±0.1de 52.8±0.4cd 15.9±0.1b Jataí IL 5.3±0.0a 0.37±0.0d 14.8±0.1ef 25.7±0.7c 0.14±0.0b 0.0±0.0e 48.0±0.5d 25.5±0.3a Mandaçaia IL 4.0±0.1d 0.14±0.0g 19.1±1.2d 32.1±0.8a 0.05±0.0b 1.0±0.0d 54.9±0.2c 6.7±0.1f Apis m IL 4.2±0.0bc 0.34±0.0d 20.0±0.8cd 18.1±0.1e 0.17±0.0b 0.0±0.0e 64.4±1.1a 10.1±0.2d Values expressed as mean ± standard deviation. a,b,c,d,e,f,g,hDifferent letters in the same column indicate significant differences between the means according to the Tukey test (p <0.05). RG: Rio Grande; GR: Gravataí; IL: Ilópolis; HMF: Hydroxymethylfurfural; F: Fructose; G: Glucose; Apis m: Apis mellifera; % m/m: mass/mass percentage. Based on Table 1, it canbeseenthathoneyfromMeliponinaebeespecieshashighermoisturecontentandlowerconcentrationofreducingsugars. Theseparameters, ifcomparedwiththeBrazilianlegislationestablished for Apismellifera, partiallymeetthequalitycharacteristics. In viewofthis, it isessentialthatthereisspecificlegislation for stinglessbees, facilitatingthecommercializationandenhancementofthemeliponicultureactivity in our country. BONTÉA, F.; DESMOULIÈREB, A. Le miel: origine et composition, Honey: origin and composition. ActualitésPharmaceutiques, v. 52, n. 531, p. 18–21, 2013. BRAZIL. MinistryofAgriculture, LivestockandSupply. NormativeInstruction No. 11, ofOctober 20, 2000. TechnicalRegulationonHoneyIdentityandQuality. MAPA, Brasília, DF, October 20, 2000. The authorsacknowledgethe financial supportgrantedbytheBrazilian agencies FAPERGS, CNPq and FINEP andfellowshipsgrantedby CAPES.

Chemical Characterization of Cupuassu (Theobroma grandiflorum L.) Pulp Extracts Using Paper Spray Mass Spectrometry

https://proceedings.science/p/120749

Priscilla do Nascimento [1]; Afonso Henrique de Oliveira Júnior [2]; Ana Luiza Coeli Cruz Ramos [3]; Yesenia Mendoza García [4]; Rodinei Augusti [5]; Mayara Neves Santos Guedes [6]; Luisa del Carmen Barrett Reina [7]; Miriã Cristina Pereira Fagundes [8]; Altamir Fernandes de Oliveira [9]; Julio Onésio Ferreira Melo [10]

[1] UFSJ- Campus Sete Lagoas (Universidade Federal de São João del-Rei - Campus Sete Lagoas); [2] Universidade Federal de São João del-Rei; [3] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [4] Universidade Federal de Alagoas ; [5] Universidade Federal de Minas Gerais; [6] Universidade Federal do Oeste do Pará; [7] Universidade Federal de Mato Grosso; [8] Universidade Estadual de Santa Cruz; [9] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [10] Universidade Federal de São João Del Rei

Innovative PS-MS methodology contributed with further understanding of the chemical complexity of extracts of cupuassu pulps, helping the identification of several molecules with diverse bioactive properties as well as their potential commercial applications in this exotic tropical fruit.

Chemical Profile Analysis of Cocoa Bean Extracts Using Solvent-Assisted Paper Spray Ionization Mass Spectrometry

https://proceedings.science/p/119939

Afonso Henrique De Oliveira Júnior [1]; Mayara Neves Santos Guedes [2]; Ana Luiza Coeli Cruz Ramos [3]; Rodinei Augusti [4]; Luisa del Carmen Barrett Reina [5]; Yesenia Mendoza García [6]; Miriã Cristina Pereira Fagundes [7]; Altamir Fernandes de Oliveira [8]; Julio Onésio Ferreira Melo [9]

[1] Universidade Federal de São João del-Rei; [2] Campus Altamira, UFPA; [3] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [4] Departamento de Química, UFMG; [5] Universidade Federal de Mato Grosso; [6] Universidade Federal de Alagoas ; [7] Universidade Estadual de Santa Cruz; [8] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [9] Universidade Federal de São João Del Rei

SAPSI-MS provided insight on characteristics of cocoa beans of pharmaceutical and medicinal relevance. This technique is a powerful tool in exploring the diversity of molecules in Brazilian flora.

Chemical profile of Annona crassiflora Mart. (Araticum) pulp by PS/MS paper spray.

https://proceedings.science/p/120406

Ana Luiza Coeli Cruz Ramos [1]; Ana Paula Xavier Mariano [1]; Afonso Henrique de Oliveira Júnior [2]; Henrique de Oliveira Prata Mendonça [3]; Priscilla Nascimento [4]; Yuri Gomes Figueiredo [5]; Rodinei Augusti [6]; Luisa del Carmen Barrett Reina [7]; Raquel Linhares Bello de Araújo [1]; Julio Onésio Ferreira Melo [8]

[1] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [2] Universidade Federal de São João del-Rei; [3] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [4] Universidade Federal de São João del-Rei / Campus Alto Paraopeba; [5] Universidade Federal de São João del Rei (campus Sete Lagoas); [6] Universidade Federal de Minas Gerais / Departamento de Química; [7] Universidade Federal de Mato Grosso; [8] Universidade Federal de São João Del Rei

The araticum proved to be an interesting fruit due to the chemical characteristics found in this word. The paper spray technical demonstrated efficient for rapid analysis of complex matrix.

Chemical Profile of Cocoa Bean Phenolic Extracts Obtained Through Solvent-Assisted Paper Spray Ionization Mass Spectrometry

https://proceedings.science/p/120030

Thaís Danielly Rocha Carneiro [1]; Afonso Henrique de Oliveira Júnior [2]; Yuri Gomes Figueiredo [3]; Mayara Neves Santos Guedes [1]; Miriã Cristina Pereira Fagundes [4]; Ana Luiza Coeli Cruz Ramos [5]; Rodinei Augusti [6]; Luisa del Carmen Barrett Reina [7]; Yesenia Mendoza García [8]; Altamir Fernandes de Oliveira [9]; Julio Onésio Ferreira Melo [10]

[1] Universidade Federal do Oeste do Pará; [2] Universidade Federal de São João del-Rei; [3] Universidade Federal de São João del Rei (campus Sete Lagoas); [4] Universidade Estadual de Santa Cruz; [5] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [6] Universidade Federal de Minas Gerais; [7] Universidade Federal de Mato Grosso; [8] Universidade Federal de Alagoas ; [9] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [10] Universidade Federal de São João Del Rei

PSI-MS approach provided novel insight into the complexity of polyphenolic extracts of cocoa beans by making it possible to identify compounds with antioxidant and bioactive properties as well as their potential commercial applications.

Comparison of non-volatile chemical species between special and traditional coffees
https://proceedings.science/p/120318

Gabriela Maria Rodrigues do Nascimento de Alcantara [1]; Wanessa Melchert Mattos [2]
[1] Centro de Energia nuclear de Agricultura-CENA/USP; [2] Universidade de São Paulo
The study evaluated the chemical composition of non-volatile species of special and traditional coffees and correlated the chemical analyzes, using principal component analysis, with their quality.

Composição metabolômica de polpa de frutos de açaí pela espectrometria de massas com ionização por paper spray
https://proceedings.science/p/119876

Thaynara da Silva Lopes [1]; Diego Maia Santos [2]; Afonso Henrique De Oliveira Júnior [3]; Henrique de Oliveira Prata Mendonça [4]; Bárbara Ventura Ferreira [5]; Mayara Neves Santos Guedes [6]; Ana Luiza Coeli Cruz Ramos [7]; Rodinei Augusti [8]; Luisa del Carmen Barrett Reina [9]; Miriã Cristina Pereira Fagundes [10]; Yesenia Mendoza García [11]; Altamir Fernandes de Oliveira [12]; Julio Onésio Ferreira Melo [13]
[1] Universidade Federal de São João del-Rei - Campus Sete Lagoas – CSL; [2] Universidade Federal de São João Del-Rei; [3] Universidade Federal de São João del-Rei; [4] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [5] Universidade Federal do Pará; [6] Universidade Federal do Oeste do Pará; [7] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [8] Universidade Federal de Minas Gerais; [9] Universidade Federal de Mato Grosso; [10] Universidade Estadual de Santa Cruz; [11] Universidade Federal de Alagoas ; [12] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [13] Universidade Federal de São João Del Rei
Metabolic composition of açaí fruit pulp by mass spectrometry with paper spray ionization. With the analyzes, the chemical composition of açaí fruit pulp was obtained, where compounds with antioxidant and bioactive properties were identified.

Cupuassu Pulp Extracts Chemical Profile Analyzed Using Paper Spray Mass Spectrometry
https://proceedings.science/p/120748

Diego Maia Santos [1]; Afonso Henrique de Oliveira Júnior [2]; Yuri Gomes Figueiredo [3]; Mayara Neves Santos Guedes [4]; Ana Luiza Coeli Cruz Ramos [5]; Rodinei Augusti [6]; Luisa del Carmen Barrett Reina [7]; Yesenia Mendoza García [8]; Miriã Cristina Pereira Fagundes [9]; Altamir Fernandes de Oliveira [10]; Julio Onésio Ferreira Melo [11]
[1] Universidade Federal de São João Del-Rei; [2] Universidade Federal de São João del-Rei; [3] Universidade Federal de São João del Rei (campus Sete Lagoas); [4] Universidade Federal do Oeste do Pará; [5] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [6] Universidade Federal de Minas Gerais; [7] Universidade Federal de Mato Grosso; [8] Universidade Federal de Alagoas ; [9] Universidade Estadual de Santa Cruz; [10] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [11] Universidade Federal de São João Del Rei
Compounds of pharmaceutical and medicinal relevance were found using PS-MS in extracts of cupuassu. This technique can be a powerful tool in exploring the diversity of molecules in Brazilian flora.

Determinação de Cd, Cr, Cu, Mn, Zn, Fe e Pb em amostras de Peumus boldus (“boldo-do-chile”) empregando a espectrometria de fluorescência de raios-X por dispersão de energia
https://proceedings.science/p/120743

Lucilia Alves Meira [1]; Janis Souza [1]; Jorge Almeida [1]; Leonardo Teixeira [1]
[1] Universidade Federal da Bahia

- Direct analysis of Peumus boldus was achieved by EDXRF.
- Time-consuming sample digestion was avoided.
- External calibration was performed with the sample matrix itself as standards.

Determination of arsenic in rice and correlation with toxic and essential elements
https://proceedings.science/p/120755

Dirce Pozebon [1]; Lucas Suchecki Barnet [1]
[1] Universidade Federal do Rio Grande do Sul

Level of As and its correlation with toxic and essential elements in rice were investigated

Toxic and essential elements (23) were determined using ICP-MS

Determination of metals from the Non-Conventional Plant Food: Bromelia antiacantha Bertol.

https://proceedings.science/p/120118

Lucélia Hoehne [1]; Marciéli Mann [1]; Aline Dalcorso [1]; Sabrina Grando Cordeiro [1]; Ytan Andreine Schweizer [1]; Bruna Costa [1]; Peterson Haas [1]; Letícia de Oliveira [1]; Gabriela Vettorello [1]; Gabriela Nunes [1]; Daiane Heidrich [1]; Elisete de Freitas [1]; Eduardo Ethur [1]

[1] Univates

Bromelia antiacantha Bertol., also known as caraguatá, carauatá, gravatá, or bananinha-do-mato, is considered an unconventional food plant (PANC). This species belongs to the *Bromeliaceae* family and is found in the South and Midwest regions of Brazil. Its cultivation has the purpose of protection and is used in the construction of hedges, but there are few studies concerning its nutritional properties. Therefore, the present study evaluated the macro and micronutrients of *B. antiacantha* fruits, in order to publicize the benefits of *B. antiacantha* for human health to intensify its consumption. Firstly, fruits were collected in the municipalities of São Francisco de Assis (BaS), Montenegro (BaM), and Guaporé (BaG), all in the state of Rio Grande do Sul, Brazil. Sample collections covered two biomes present in the state: the Pampa (São Francisco de Assis) and the Atlantic Forest (Guaporé and Montenegro), throughout May and June 2019. Samples were collected, weighed, and frozen. Subsequently, acid digestion of samples occurred in a microwave and the analyzes were made by atomic absorption spectrometry in a graphite oven and flame atomic absorption spectrometry to determine fruit metals. The results indicated that *B. antiacantha* contains high levels of Ca (65-72 mg / 100 g), K (212-258 mg / 100 g) and Mg (48-83 mg / 100 g). Moreover, it revealed higher levels of Zn, Mn, Fe, and Ni regarding other vegetables, such as pineapple and broccoli, for example. Upcoming procedures include bioaccessibility analysis of these metals, in order to provide more information to consumers. Therefore, *Bromelia antiacantha* Bertol. contains essential nutrients to the human organism, which can contribute to a greater diversity of natural foods.

Determination of the inorganic profile of teas derived from Camellia Sinensis.

https://proceedings.science/p/119792

Ana Flávia Loureiro Martins Nascimento [1]

[1] UENF

Development of an in vitro digestion model and of an analytical method to assess the bioaccessibility of bromine and iodine in edible seaweeds

https://proceedings.science/p/119565

Priscila Tessmer Scaglioni [1]; Fernanda Pitt Balbinot [1]; Filipe Soares Rondan [1]; Diogo la Rosa Novo [1]; Bruna Holz Xavier [1]; Marcia Mesko [1]

[1] Universidade Federal de Pelotas

The bioaccessible fractions of Br and I vary according to seaweed species. The total concentration of Br and I in edible seaweeds may not represent the bioaccessible fraction in the human organism.

Evaluation chemical compounds of araticum using mass spectrometry (paper spray).

https://proceedings.science/p/120746

Jéssica da Silva Dias [1]; Ana Luiza Coeli Cruz Ramos [2]; Afonso Henrique De Oliveira Júnior [1]; Ana Paula Xavier Mariano [3]; Henrique de Oliveira Prata Mendonça [4]; Yesenia Mendoza García [5]; Rodinei Augusti [3]; Mayara Neves Santos Guedes [6]; Luisa del Carmen Barrett Reina [7]; Miriã Cristina Pereira Fagundes [8]; Altamir Fernandes de Oliveira [9]; Raquel Linhares Bello de Araújo [3]; Julio Onésio Ferreira Melo [10]

[1] Universidade Federal de São João del-Rei; [2] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [3] Universidade Federal de Minas Gerais; [4] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [5] Universidade Federal de Alagoas ; [6] Universidade Federal do Oeste do Pará; [7] Universidade Federal de Mato Grosso; [8] Universidade Estadual de Santa Cruz; [9] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [10] Universidade Federal de São João Del Rei

The present study shows great efficiency and potential of the technique in identifying the compounds. It also contributes to greater knowledge about the fruit, its characteristics, and chemical compounds that can add higher value to the product.

Evaluation of the hydrogen peroxide detection limit in milk based on the official qualitative analysis methodology

https://proceedings.science/p/119447

João Paulo Victorino Santos [1]; Simone Machado Goulart [1]; Thainá Souza Santos [2]; Henrique Faria Paula [2]; Leonardo Castro [3]

[1] Instituto Federal de Ciência e Tecnologia de Goiás / IFG; [2] IFG; [3] IFG-Campus Itumbiara

Hydrogen peroxide is used in milk as an inhibitor of bacterial growth. Your presence is a fraud. The official qualitative analysis methodology does not indicate the detection limit of the method.

Extensão Universitária: Oficinas de produção de sabão em comunidades periféricas da cidade de Marabá-PA

https://proceedings.science/p/119648

Aline Maria Viana de Souza [1]; Tatiani da L. Silva [2]; Elieuda dos Reis Santos [3]; Jefferson Carlos Dias Vieira [3]

[1] Universidade do Estado do Pará; [2] 2Universidade Federal do Sul e Sudeste do Pará ; [3] Universidade do Estado do Pará--Campos VIII/Marabá

Tratar ou destinar corretamente os resíduos urbanos é uma responsabilidade da qual a sociedade vem cada vez mais tomando consciência, sendo uma questão de cidadania propor alternativas para que estes rejeitos causem o menor impacto ambiental possível. Assim, aliando o conhecimento dos impactos ambientais causados pelo descarte inadequado de óleo de cozinha nos leitos dos rios da cidade de Marabá-PA e do conhecimento das possíveis alternativas de minimização dos impactos ambientais agregado ao conhecimento químico do que ocorre em tais processos, buscou-se realizar um processo de conscientização ambiental com donas de casas de comunidades periféricas da cidade e promover oficinas de produção de sabão utilizando como obra prima o óleo de fritura que seria descartado.

Infrared spectroscopy and chemometrics tools applied to edible oils characterization

https://proceedings.science/p/120591

Carlos Guilherme Tissi Batista [1]; Cibele Maria Stivanin de Almeida [1]

[1] Universidade Estadual do Norte Fluminense Darcy Ribeiro

- ATR-FTIR technique acquired the mid-infrared spectra of linseed, sunflower, rapeseed, corn and soybean oils.
- The classification does not classify some commercial linseed oils as linseed oil class.

PERFIL DE COMPOSTOS ORGÂNICOS VOLÁTEIS POR SPME/MS EM MANTEIGA GHEE

https://proceedings.science/p/120745

Tassia Nunes de Albuquerque Rodrigues [1]; Ana Luiza Coeli Cruz Ramos [2]; Ana Paula Xavier Mariano [1]; Rodinei Augusti [1]; Luisa del Carmen Barrett Reina [3]; Raquel Linhares Bello de Araújo [1]; Julio Onésio Ferreira Melo [4]

[1] Universidade Federal de Minas Gerais; [2] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [3] Universidade Federal de Mato Grosso; [4] Universidade Federal de São João Del Rei

Profile of volatile organic compounds by SPME/MS in Manteiga ghee. Identification of volatile in manteiga ghee by headspace mode solid phase microextraction (HS-SPME), obtaining chemical compounds.

PERFIL DE COMPOSTOS ORGÂNICOS VOLÁTEIS POR SPME/MS EM SEMENTES DE AROEIRA DO SERTÃO

https://proceedings.science/p/119613

Yuri Gomes Figueiredo [1]; Laiza Andrade Nogueira [2]; Ana Luiza Coeli Cruz Ramos [3]; Rodinei Augusti [4]; Luisa del Carmen Barrett Reina [5]; Yesenia Mendoza García [6]; Mayara Neves Santos Guedes [2]; Altamir Fernandes de Oliveira [7]; Miriã Cristina Pereira Fagundes [8]; Julio Onésio Ferreira Melo [9]

[1] Universidade Federal de São João del Rei (campus Sete Lagoas); [2] Universidade Federal do Oeste do Pará; [3] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [4] Universidade Federal de Minas Gerais; [5] Universidade Federal de Mato Grosso; [6] Universidade Federal de Alagoas ; [7] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [8] Universidade Estadual de Santa Cruz; [9] Universidade Federal de São João Del Rei

Profile of volatile organic compounds by SPME/MS in Aroeira do Sertão seeds. Identification of volatile aroeira seed compounds by headspace mode solid phase microextraction (HS-SPME), obtaining chemical compounds from the monoterpenes and sesquiterpenes class.

PERFIL QUÍMICO DE AÇAÍ, POR ESPECTROMETRIA DE MASSAS USANDO IONIZAÇÃO AMBIENTE EM PAPER SPRAY, NO MODO NEGATIVO.

https://proceedings.science/p/119674

Afonso Henrique de Oliveira Júnior [1]; Diego Maia Santos [2]; Henrique de Oliveira Prata Mendonça [3]; Yuri Gomes Figueiredo [4]; Bárbara Ventura Ferreira [5]; Mayara Neves Santos Guedes [6]; Ana Luiza Coeli Cruz Ramos [7]; Rodinei Augusti [8]; Luisa del Carmen Barrett Reina [9]; Miriã Cristina Pereira Fagundes [10]; Yesenia Mendoza García [11]; Altamir Fernandes de Oliveira [12]; Julio Onésio Ferreira Melo [13]

[1] Universidade Federal de São João del-Rei; [2] Universidade Federal de São João Del-Rei; [3] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [4] Universidade Federal de São João del Rei (campus Sete Lagoas); [5] Universidade Federal do Pará; [6] Universidade Federal do Oeste do Pará; [7] Universidade Federal de Minas Gerais / Faculdade de Farmácia / Departamento de Alimentos; [8] Universidade Federal de Minas Gerais; [9] Universidade Federal de Mato Grosso; [10] Universidade Estadual de Santa Cruz; [11] Universidade Federal de Alagoas ; [12] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [13] Universidade Federal de São João Del Rei

Chemical profile of açaí, by mass spectrometry using ambient ionization in paper spray, in negative mode. The PSI-MS approach provided new information on the complexity of the polyphenolic extracts of açaí fruit pulp, enabling the identification of compounds with antioxidant and bioactive properties.

Portable near-infrared spectroscopy and multivariate calibration applied to the determination of alcohol content in beers

https://proceedings.science/p/120017

Marcelo Sena [1]

[1] UFMG

Rapid and low cost determination of total Hg in cat foods by photochemical vapor generation coupled to atomic absorption spectrometry

https://proceedings.science/p/119630

Gisele Simone Lopes [1]; Nilvan Alves Silva [1]; Nandressa Felipe Nobre [1]
[1] Universidade Federal do Ceará

A rapid and low-cost method for determination of total mercury (THg) in cat food was developed based on photochemical vapor generation (PVG) coupled to cold vapor atomic absorption spectrometry (CVAAS). Cat food samples with ingredients based on tuna fish and other seafood were investigated. Organic acid precursor and concentration for radical generation and Hg photoreduction, sample UV irradiation time, and carrier gas flow were optimized. Highest PVG efficiency was achieved using 10% v v−1 formic acid, 4-s UV irradiation time, and a carrier gas flow of 50 mL min−1. The calibration function presented a correlation coefficient of 0.99. Accuracy was confirmed by analysis of Certified Reference Materials with recoveries of 93–110% and relative standard deviation lower than 6%. Under optimized conditions, a procedural detection limit of 0.28 µg kg−1 was obtained. Determination of THg in 10 samples of cat food purchased in local markets revealed a concentration range of 0.035–0.388 mg kg−1. Highest concentrations were found in cat foods. Only one sample presented a concentration close to the regulatory limit of the European Commission Directive. Assuming the estimated daily food intake (EDI) calculated in a range of 0.0021 to 0.023 mg of THg per day per kg body weight, it is concluded that it remains below that considered lethal for cats. The methodology is efficient, simple, low cost, and fit for purpose.

Reconhecimento do potencial hepatoprotetor baseado em PCA: correspondências em Solanum paniculatum L.

https://proceedings.science/p/120179

Juliane Xavier dos Santos [1]; Simone de Oliveira Santos [1]; Tiago Branquinho Oliveira [1]
[1] Universidade Federal de Sergipe

PCA-based hepatoprotective potential recognition: Solanum paniculatumL matching: This work aimed to identify substances with hepato protective potential of the species Solanum paniculatum L. from the PCA analysis.

Sodium hydroxide in milk: detection limit based on the official qualitative analysis methodology.

https://proceedings.science/p/119429

Simone Machado Goulart [1]; João Paulo Victorino Santos [1]; Thainá Souza Santos [1]; Henrique Faria Paula [1]; Leonardo Castro [2]
[1] Instituto Federal de Ciência e Tecnologia de Goiás / IFG; [2] IFG-Campus Itumbiara

Sodium hydroxide is used in milk as an acidity reducer. Your presence is a fraud. The official qualitative analysis methodology does not indicate the detection limit of the method.

Successive digestions of honey for pre-concentration of bromine for further determination by ion chromatography with mass spectrometry

https://proceedings.science/p/120140

Fernanda Pitt Balbinot [1]; Priscila Tessmer Scaglioni [1]; Filipe Soares Rondan [1]; Álisson Aline da Silva [1]; Cláudio Alves Lima Junior [1]; Cleiton J. Andrade Pereira [1]; Marcia Mesko [1]
[1] Universidade Federal de Pelotas

A method for Br determination in honey by IC-MS was developed. Successive digestions of high sample masses of honey (3.2 g) were possible using MIC. A six-fold reduction in the LOQ has been achieved.

The use of simulated gastric digestion in order to assure mineral nutrition quality in small and medium size psittacines pet food.

https://proceedings.science/p/119663

Filipi Chalita Guimarães [1]
[1] Universidade Estadual do Norte Fluminense Darcy Ribeiro

Catálise - CAT

A combined computational and experimental study on Suzuki-Miyaura reaction catalyzed by N,N'-Bridged Binuclear NHC Palladium Complexes: what is the active catalyst?

https://proceedings.science/p/120620

Natalia Lussari Vrech [1]; Ataualpa Braga [1]; Ming-Tsz Chen [2]
[1] Universidade de São Paulo; [2] Providence University

Bipalladium NHC nitrogen-based alkyl chain ligands starting catalysts. Experimental and theoretical kinetic analysis. Mono vs. binuclear Pd mechanism.

Biodiesel Production from Palm Fatty Acid Distillate Using Carbon-based Catalyst from Spent ground Coffee

https://proceedings.science/p/119448

Ana Paula da Luz Corrêa [1]; Paula Maria Melo da Silva [1]; Joselia Alves de Almeida Silva [1]; Rafael Roberto Cardoso Bastos [1]; Dayenne Alexsa Araujo de Souza [1]; Matheus Arrais Gonçalves [1]; GERALDO Narciso da Rocha Filho [1]; Leyvison Rafael Vieira da Conceição [1]
[1] UFPA

Palm fatty acid distillate (PFAD) is a non-desired by-product from the crude palm oil refinery process. Thus, the present study aims to synthesize an acid catalyst from spent ground coffee and to apply it in the esterification reaction of PFAD for biodiesel production, as well as to optimize the reaction conditions. The spent ground coffee was carbonized in a tubular oven at 600 °C for 1 h, with nitrogen flow of 80 mL min-1. The obtained biochar (BC) was sulfonated using 1.0 g of BC and 10 mL of concentrated H2SO4 (ratio 1:10), at 200 °C for 4 h. After, the solid was washed with deionized water to neutral pH and kiln-dried at 60 °C for 24 h to obtain the catalyst with a total acid density of 5.54 mmol H+ g-1. The response surface methodology was based on an experimental design of Box & Behnken and it was used to obtain the best reaction conditions. The coefficient of determination (R2) has showed adequate (0.91608), indicating the percentage of experimental variance explained by the proposed regression equation. The conversion of reaction products was determined by the evaluation of acid values, according to AOCS Cd 3d-63 standard. The best reaction conditions obtained in the optimization for time, temperature and catalyst concentration were 2 h, 120 °C and 3.5%, respectively, with a conversion of 97.2%. The reaction between methanol and PFAD without catalyst shows a conversion of 16.9%, while the reaction uses only BC as a catalyst was 19.7%, what demonstrate the high catalytic performance of this type of (acid) catalyst. According to the pareto diagram and response surface methodology, temperature is a factor that considerably influences the conversion rates of FFA to methyl ester.1 In the studied levels of temperature (60–120 °C) and time (0,5–2,5 h), the best values for biodiesel conversion are obtained for the highest points. In this way, low concentrations of catalyst (around 3%) are capable of promoting high conversion rates (>90%) for times from 2 h and for temperatures from 100 °C. The catalyst remained highly efficient at its first reuse: 89.6% (conversion). Thus, the results revealed a promising utilization for spent ground coffee as a sustainable feedstock for the synthesis of a heterogeneous acid catalyst in the biodiesel production from PFAD. 1 .ALHASSAN, Fatah H. et al. Applied Catalysis A: General, v. 456, p.182-187, 2013.

Catalisadores de metais nobres suportados em Nb2O5 para valorização da xilose

https://proceedings.science/p/120228

Paola Caroline de Oliveira [1]; Simone de Jesus Canhaci [2]; Catarine B. Gabriel [2]; Andréa Maria Duarte de Farias [3]; Marco A. Fraga [3]

[1] Instituto Militar de Engenharia; [2] INT (Instituto Nacional de Tecnologia); [3] Instituto Nacional de Tecnologia - INT

Xylose upgrading over Nb2O5-supported noble metals catalysts. Niobium based materials are promising catalysts for xylose conversion.

Catalytic activity of mixed oxides in the conversion of xylose to obtain chemical inputs

https://proceedings.science/p/119762

Débora Olimpio da Silva Avelino [1]; Thatiane Veríssimo dos Santos [2]; Dhara Beatriz de Amorim Pryston [1]; Mario Roberto Meneghetti [3]; Simoni Margareti Plentz Meneghetti [1]

[1] Universidade Federal de Alagoas, Grupo de Cátalise e Reatividade Química, Instituto de Química e Biotecnologia.; [2] Universidade Federal de Alagoas, Grupo de catálise e Reatividade Química e Instituto de Química e Biotecnologia.; [3] Universidade Federal de Alagoas

Catalytic performance of heterogeneous catalysts in the conversion of xylose in order to obtain chemicals of high industrial interest.

Catalytic Performance and Deactivation of Sulfonated Biochar in the Biodiesel Production from Amazon Oils: Decisive Role of Chlorophyll Content

https://proceedings.science/p/119655

Rafael Roberto Cardoso Bastos [1]; ANA PAULA DA CORREA [1]; Patrícia Teresa Souza da Luz [2]; GERALDO Narciso da Rocha Filho [1]; José Roberto Zamian [1]; Leyvison Rafael Vieira da Conceição [1]

[1] UFPA; [2] IFPA

Murumuru kernel shell, an agro-industrial waste, was used as the precursor biomass in the synthesis of an acid biochar that was employed as a catalyst in the production of biodiesel originated from jupati oil. The catalyst was synthesized from the carbonization of murumuru kernel shell, followed by sulfonation in concentrated sulfuric acid. It was characterized by an acid-base titration in order to determine total acid density, X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), fourier transform infrared (FT-IR) spectroscopy, and thermogravimetric analysis (TG). The used condition for temperature, catalyst concentration, and methanol/oil molar ratio in jupati biodiesel production were 135 °C, 6% and 30:1, respectively. It also reached an ester content of 91.8%. During catalyst reuse tests based on crude jupati oil, an abrupt drop in its catalytic activity was observed: around 65% for the second reaction cycle, when compared to the first cycle. We chose to use the same industrial waste as raw material and as an alternative adsorbent to remove the chlorophyll contaminant from crude jupati oil in order to synthesize sulfonated biochar from murumuru kernel shell biochar. With the synthesized material, it was possible to remove about 92.5% of the initial chlorophyll present (12.4 ppm). The results of the study on catalytic reuse for purified jupati oil showed that catalyst deactivation after the first reaction cycle occurred due to the high chlorophyll concentration of crude jupati oil. The catalyst achieved catalytic activity at around 80% in terms of ester content for the fourth cycle using the purified oil. Thus, proposing the acid solid from the murumuru kernel shell as a bifunctional material in the removal of chlorophyll from vegetable oils and acid catalysis for biodiesel production. Additionally, successive reactions were performed with buriti oil, which has low chlorophyll concentration (close to 0.1 ppm). Thus, we could attest that the deactivation of sulfonated biochar occurs by means of chlorophyll adsorption during the first reaction cycle. The values of ester content for the study of catalyst reuse with buriti oil prove that no deactivation of the heterogeneous acid catalyst can be found in successive esterification-transesterification reactions using an oil source with low chlorophyll content since it maintains a performance and catalytic stability very similar to that found for the purified jupati oil investigated in this study. The catalytic activity of catalyst gradually decreases with reuse, maintained the catalytic activity around 80% of ester content until the fourth reaction cycle using purified jupati oil and buriti oil. This catalytic activity reduction is mainly attributed to the leaching of active sites (-SO3H). The reusing and ester content results found in this study showed that the chlorophyll content plays a decisive role in the choice of lipid matrices for the biodiesel production, because this bioactive can deactivate catalytic sites by adsorption resulting in blocking of active sites, impairing the catalytic performance in successive reaction cycles for this type of catalyst (BASTOS et al., 2020). BASTOS, R. R. C. et al. Optimization of biodiesel production using sulfonated carbon-

based catalyst from an amazon agro-industrial waste. Energy Conversion and Management, v. 205, n. October 2019, p. 112457, 2020.

CO2 fixation into cyclic carbonates under supercritical conditions catalyzed by a carbon-based material derived from Zinc Tetraphenylporphyrin

https://proceedings.science/p/120294

Nágila El Chamy Maluf [1]; Pedro Miguel Vidinha Gomes [1]; Liane Rossi [1]
[1] IQ-USP

CO2 is the most abundant waste produced by human activities and a greenhouse gas in the atmosphere. On the other hand, CO2 is also non-toxic, renewable and cheap carbon source. Among innumerous CO2 valorization reactions, its insertion in epoxides is an attractive way due the formation of two different, yet valuable, products: cyclic (CC) and polymeric carbonates (PC). Many catalysts for the cycloaddition of CO2 to epoxides are represented by binary systems with the Lewis acidic component being denoted as the “catalyst” and the nucleophilic component as the “co-catalyst”. The Lewis acidic catalysts are not active in the absence of a nucleophilic co-catalyst. Herein, we prepared a single-component catalyst displaying both components in a multifunctional carbon-based material. Firstly, we synthesize zinc tetraphenylporphyrin and phthalocyanine (ZnTPP and ZnPc, respectively) and then they were pyrolysed at 800 °C for 2 hours under N2 atmosphere, trying to obtain N and Zn atoms doped carbon materials. These samples were called ZnTPP_800C and ZnPc_800C. These materials are being characterized by UV-Vis, XPS, XRD, elemental analysis (CHN), ICP OES, TEM, TGA and BET. The reactions were performed in a batch reactor under CO2 supercritical (scCO2) conditions. The results are revealed in Table 1. So far, no co-catalyst has been applied yet showing that the ZnTPP_800C probably has nucleophilic and Lewis acid sites. This reaction had been hardly ever studied in scCO2. In this work, this condition was fundamental in selectivity to organic CC, suppressing all the possible polymerization reactions.

Cyanosilylation Reaction Catalyzed by Lanthanide Frameworks (Ln-MOFs).

https://proceedings.science/p/120085

Lucas Queiroz dos Santos [1]; Jonathan Christoff Martins Antônio [1]; Cristiane Kelly de Oliveira [1]; Ivani Malvestiti [1]
[1] Universidade Federal de Pernambuco

Solvent-free cyanosilylation reaction presented aldehyde selectivity for the catalyst [La(2-MeSBz)3]. The reaction with ketones afforded low to moderated yields only with [Eu2(Fum)3(H2O)4]n ·3H2O.

EDTA-FUNCTIONALIZED CHITOSAN: NEW AND EFFICIENT HETEROGENEOUS CATALYST IN THE KNOEVENAGEL CONDENSATION AT ROOM TEMPERATURE

https://proceedings.science/p/119783

Paloma Gomes de Abrantes [1]; Israel Ferreira da Costa [1]; Ercules Epaminondas de S. Teotonio [1]; Juliana Alves Vale [1]
[1] Universidade Federal da Paraíba

Chitosan of low (LWC) and medium (MWC) weight were functionalized with EDTA. Quick and efficient catalyst in the Knoevenagel Condensation at room temperature.

Effect on the textural properties of cobalt in Al2O3/CeO2 and its catalytic properties in the BTX oxidation reactions

https://proceedings.science/p/120455

Rosana Balzer [1]; Anderson Schwanke [2]
[1] Universidade Federal do Paraná – Campus Palotina; [2] Universidade Federal do Rio Grande do Sul

BTX’s are considered to be a major contributor to air pollution. The catalysts Co/Al2O3-CeO2 were prepared. The catalytic activity of the catalysts was studied in the oxidation of BTX

Enzymatic resolution synthesis of enantiomerically pure acetate esters from aliphatic monoalcohols in the preparation of flavor esters

https://proceedings.science/p/120420

Calionara Waleska Barbosa Melo [1]; Raquel Ana Apela Leão [1]; Rodrigo Octavio Mendonça Alves de Souza [1]; Claudia Moraes de Rezende [1]

[1] Universidade Federal do Rio de Janeiro

Lipase N435 preferably formed the enantiomer R of the acetate esters. Esters start to form after the first two hours of reaction. For alcohols 1a and 1d, the S enantiomer of esters, were formed afte

Fatty acid esterification over mesoporous [Al]-SBA-15 catalysts

https://proceedings.science/p/119763

Marco A. Fraga [1]; Simone Canhaci [1]; Elise Mota de Albuquerque [1]; Andréa Maria Duarte de Farias [1]; Camila Lopes [1]; Cristina Quitete [2]; Silvino Chinelatto [2]

[1] Instituto Nacional de Tecnologia - INT; [2] Petrobras

[Al]-SBA-15 is an efficient and stable catalyst for fatty acid esterification.

g-C3N4 em Reações do Tipo Fenton Heterogêneo

https://proceedings.science/p/120037

Wanessa Lima de Oliveira [1]; Meirielle A. Ferreira [1]; Pedro B. C. Serra [1]; Henrique A. J. L. Mourão [1]; Manoel J. M. Pires [1]; Walker Vinícius Ferreira do Carmo Batista [2]; Honória F. Gorgulho [2]; Daniel F. Cipriano [3]; Jair C. C. Freitas [3]; Valmor R. Mastelaro [4]; Dalva Ester da Costa Ferreira [1]; Frederico R. Fioravante [1]; MARCIO CESAR PEREIRA [1]; João Paulo Mesquita [1]

[1] UFVJM; [2] UFSJ; [3] UFES; [4] USP

O processo Fenton tradicional apresenta algumas desvantagens, tais como a perda de estabilidade em pH superior a 3 e a formação de resíduos1,2. Estes problemas têm motivado o desenvolvimento de catalisadores heterogêneos, em sistemas conhecidos como Fenton heterogêneo, que além de buscar uma otimização do processo tradicional, visa o desenvolvimento de novos catalisadores baseados em materiais livres de metais (Do inglês: metal-free), devido ao alinhamento deste conceito de catalisador com àqueles relacionados com a "Química Verde" (do inglês: Green chemistry), a qual visa garantir o desenvolvimento industrial por meio de ações ecologicamente menos prejudiciais ao meio ambiente3 . Neste contexto, temse o nitreto de carbono grafítico (g-C3N4), um material sem toxicidade e que devido à ampla disponibilidade de seus constituintes, baixo custo, facilidade de preparação e estrutura de bandas posicionada adequadamente para a foto-oxidação e redução de moléculas de água4 , tornou-se alvo de diversos estudos. Desta maneira, neste trabalho nós mostramos o uso g-C3N4 como catalisador para reações do tipo Fenton heterogêneo, a princípio ainda não relatado na literatura. Os g-C3N4 foram obtidos através da policondensação da melamina em diferentes temperaturas finais de condensação (300, 350, 400, 450, 500, 550 e 600 °C). Todos os materiais foram caracterizados por diferentes técnicas incluindo DRX, FTIR, CHN-O e XPS. As atividades catalíticas tipo Fenton heterogêneo foram avaliadas a partir do monitoramento com a Espectroscopia UV-Vís da descoloração do corante índigo carmim (10 mg L-1) na presença de 15 mg de g-C3N4 e 25 µL de H2O2 (34% m/m). Os g-C3N4 obtidos nas temperaturas de 500 a 600 ° C foram capazes de promover a descoloração do corante, assim, com base em uma extensa caracterização destes materiais, cálculos teóricos e o conjunto de resultados obtidos, acredita-se que grupos funcionais oxigenados reduzidos, tais como, C-OH e/ou –NH-OH, provavelmente formados durante a condensação térmica da melamina nas temperaturas entre 500 e 600 °C, são capazes de formar radicais hidroxilas na presença de H2O2, como mostrado pela Ressonância Paramagnética Eletrônica. Desta maneira, concluímos que a reatividade deste material está diretamente relacionada à estrutura única do gC3N4 em associação com grupos funcionais oxigenados presentes em sua superfície. Neste âmbito, além de novas informações sobre a reatividade da superfície do g-C3N4, estes resultados podem contribuir para pesquisas relacionadas ao uso do g-C3N4 como catalisador em diferentes reações de oxidação.

Gold-amine-catalyzed transfer hydrogenation of alkynes with formic acid

https://proceedings.science/p/120306

Liane Rossi [1]
[1] IQ-USP

We explored formic acid as a hydrogen source for transfer hydrogenation catalyzed by gold. The key to success is the use an appropriate amine, which acts cooperatively with the gold surface. In this talk, the development of gold catalysts in our research group will be revised, either with H2 and HCOOH.

Heterogeneous acid catalyst based on iron ore tailings for biodiesel synthesis

https://proceedings.science/p/119995

Caroline Duarte Prates [1]; Rochel Montero Lago [1]; Ana Paula de Carvalho Teixeira [1]
[1] Universidade Federal de Minas Gerais

Heterogeneous acid catalyst based on sulfated iron oxide; mining waste was used as a source of iron oxide; catalyst use on esterification of oleic acid and methanol showed promising results.

Hierarchical β-zeolites for the valorization of furfural via domino reaction

https://proceedings.science/p/120598

Thiago de Melo Lima [1]; Leyliane Greyce dos Santos Batinga [1]; Luiz Felipe Couto Pinhel [1]; Sancler Vasconcelos [1]; Vinicius Rossa [1]
[1] Universidade Federal Fluminense

Hierarchical beta zeolites were prepared by dealumination and desilication protocols and used as a catalyst for the furfural conversion to isopropyl levulinate.

Hydrogenolysis and dehydrogenation of cyclohexane using Nickel Aluminate as precursor: Effect of the concentration of NiAl2O4

https://proceedings.science/p/120232

Aracelis Jose Pamphile Adrian [1]; Fabio Passos [2]; Pedro Pablo Florez Rodriguez [1]
[1] Instituto de Química e Biotecnologia, Universidade Federal de Alagoas; [2] Departamento de Engenharia Química e de Petróleo, Universidade Federal Fluminense

Hydrogenolysis and dehydrogenation of cyclohexane using nickel aluminate as precursor: effect of NiAl2O4 concentration. A maximum of 16wt.% of Ni is inserted in the structure. NiAl2O4 is an interesting precursor for C-C and C-H cleavage reactions and allows control of particle size.

Imobilização da Amano Lipase de Mucorjavanicus em suporte hidrofóbico via adsorção física

https://proceedings.science/p/120084

Eliézer Luz do Espirito Santo [1]; Marta Maria Oliveira dos Santos [2]; Luiz Henrique Sales de Menezes [3]; Marise Silva de Carvalho [1]; Adriano Aguiar Mendes [4]; Julieta de Oliveira [1]; Marcelo Franco [1]
[1] Universidade Estadual de Santa Cruz; [2] Universidade Estadual do Sul da Bahia; [3] Departamento de Ciências Exatas e Tecnológicas, Universidade Estadual de Santa Cruz - UESC, Ilhéus, Brasil; [4] Instituto de Química (UNIFAL) / Universidade Federal de Alfenas

Immobilization of Amano Lipase from Mucorjavanicus on hydrophobic support via physical adsorption.Scanning electron microscopy (SEM) in the characterization of Diaion HP 20;

Layered double hydroxides as catalysts for the synthesis of scaffolds for solar cells

https://proceedings.science/p/120114

Jaqueline Senra [1]; Matheus Lopes Modena [2]; Lorenna Conti Loffredo Luscura França da Silva [2]; Luiz Fernando Brum Malta [2]

[1] UNIVERSIDADE DO ESTADO DO RIO DE JANEIRO; [2] UNIVERSIDADE FEDERAL DO RIO DE JANEIRO

Highlights

- Aryl thiophenes were prepared as starting materials for the design of π-extended conjugated dyes.
- Layered double hydroxides were used as catalysts and allowed yields up to 98%.

Solar cells are considered the most promising energy devices for the future energy demands. Most of them are silicon-based solar cells, which have power conversion efficiencies (PCEs) of over 20% but disadvantages such as high cost, limited tunability and environmental issues. Therefore, efforts have been considered in order to improve organic photovoltaic technologies. In this case, the typical photoactive layer is based on low band gap small molecules electron donors combined with electron acceptors. In the last few years, layers composed of electron push and pull structures have allowed easier energy level control and improved PCEs. Aryl thiophenes and derivatives are considered privileged bridges to link donor and acceptor units because of their great impact on the overall optical and charge transport properties. In this work, we aimed to show preliminary results concerning the synthesis aryl thiophenes as potential starting materials for the design of π-extended conjugated dyes. Based on previous results reported by our group [2], we explored the use of Pd impregnated on Cu/Al layered double hydroxide (LDH) as catalysts for the Suzuki-Miyaura reaction. The synthesis of Cu/Al LDH followed the work previously described [2]. Then, the material was impregnated with Na2PdCl4 in DMF, resulting in the formation of PdNPs. Analysis of the material by SEM-FEG and XPS indicated the formation of nanoparticles with a mean size distribution of 20-35 nm and Pd(0): Pd(II) = 65:35. Initial results for the Suzuki-Miyaura reaction between 2-iodothiophene and arylboronic acids, revealed a good catalyst efficiency under mild conditions. For instance, the use of 9,9-dimethyl-fluoreneboronic acid allowed a moderate yield under only 0.5 eq. of base, suggesting the participation of the HDL surface in the reaction outcome. Analysis of electronic and steric effects are underway. [1] MAY, L. et al. Org. Chem. Front. 2019, 10.1039/c9qo01318k. [2] Silva, L.C.L.L.F. et al. Catalysts 2019, 9, 301.

METAL OXIDES EMPLOYED AS HETEROGENEOUS CATALYSTS IN THE ISOMERIZATION OF GLUCOSE IN AQUEOUS MEDIA.

https://proceedings.science/p/119516

Evellyn Patricia Santos da Silva [1]; Thatiane Veríssimo dos Santos [2]; Simoni Margareti Plentz Meneghetti [1]

[1] Universidade Federal de Alagoas; [2] Universidade Federal de Alagoas, Grupo de catálise e Reatividade Química e Instituto de Química e Biotecnologia.

Metal oxides were used as heterogeneous catalysts;
Mild temperature (70°C) was used for the catalytic tests;
Acid sites of metal oxides favored conversions and yields to fructose.

Modified BEA zeolite applied on dehydration of xylose to furfural

https://proceedings.science/p/119461

Maria Clara Hortencio Clemente [1]; Deborah da Silva Valadares [1]; Gesley Alex Veloso Martins [1]; Sílvia Cláudia Loureiro Dias [1]; JOSÉ ALVES DIAS [1]

[1] Universidade de Brasília

The biomass processing industry is becoming increasingly interesting from the environmental point of view, since it is used as a feedstock that is underused or discarded from the sugar and alcohol industries. Thus, many efforts have been directed towards obtaining chemicals from the processes of valorization of these residues. Furfural, which is considered a building block of several other molecules of chemical, pharmaceutical and food industry interest, is one that is produced from biomass. Its production from biomass occurs through the acidic hydrolysis of hemicellulose like pentosans generating C5 chain sugars such as xylose. Then, the sugar is dehydrated and the furfural product is obtained. In order for the balance of hydrolysis reactions to be reached more quickly, acid catalysts are normally used. This is so far the most effective and cheapest way to obtain furfural from biomass. In order to optimize the chemical

reactions and waste generated, heterogeneous catalysts have been studied in the dehydration of sugars such as xylose.

Photocatalytic performance of the BiVO4@TiO2 heterojunction against degradation of methylene blue dye

https://proceedings.science/p/119532

Luis Henrique Segantini [1]; Roberto de Matos [1]; Caroline Santana dos Santos [1]; Roberta Antigo Medeiros [1]; Marcelo Zampieri [1]; Yuri Vinicius Bruschi de Santana [2]; Raul Zanchet [1]; Rafael Junqueira Leal [1]
[1] Universidade Estadual de Londrina; [2] Universidade Tecnológica Federal do Paraná

Synthesis of BiVO4@TiO2 by the microwave hydrothermal method, presence of crystalline phases with greater photoactivity.
High photocatalytic property of BiVO4@TiO2 degrading 83% of the dye (MB).

Ruthenium(II)-Nickel(II) heterobimetallic catalyst for ROMP and ethylene polymerization

https://proceedings.science/p/119478

Gustavo Henrique Cicero Masson [1]; Patrik Gois [1]; Daniele Martins [2]; Benedito Neto [2]; Beatriz Eleutério Goi [3]; Valdemiro Pereira de Junior [3]
[1] Departamento de Física, Química e Biologia / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade de São Paulo; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"
The polymerization of ethylene is initiated by coordinating the olefin in the mono-alkylated metal complex in the vacant site to initiate the propagation forming a saturated polymer. Whereas the ROMP is a kind of metathesis between cyclic olefins, which is catalyzed by the metal-carbene complex [LnM=CHR], providing an unsaturated polymer. These two polymerization methods are catalyzed by different catalytic systems. Here, the complex [(N,O)Ni(PPh3)Cl – Ru(p-cymene)] was synthetized as multifunctional catalyst to mediate both the reactions (ROMP and ethylenepolymerization). The Ru-Ni bimetallic complex was characterized by FTIR, UV-Vis and 1H, 13C{1H} and 31P{1H} NMR. The synthetized complexes were evaluated on ROMP reaction using norbornene (NBE) under conditions of [EDA]/[Ru] = 28 (15 L) and [NBE]/[Ru] = 3500 for 60 min at 323.15 K, getting a conversion about 38% after 60 minuts. Ethylene polymerization using similar complex based on monometalic Ni(II) specie with Schiff base [N,O-Ni(PPh3)Cl] has been reported in the literature showing high catalytic activity in the presence of methyaluminoxane (MAO) as co-catalyst. Thus, the catalytic tests for bimetallic complex on ethylene polymerization is in progress.

Ruthenium-palladium heterobimetallic complex as a multifunctional catalyst for ROMP and ethylene polymerization

https://proceedings.science/p/119483

Patrik Dione de Santana Gois [1]; Gustavo Henrique Cicero Masson [2]; Juliana Iris P. Maia [3]; Daniele Martins [4]; Pedro Ivo da Silva Maia [3]; Benedito Neto [4]; Beatriz Eleutério Goi [1]; Valdemiro Pereira de Junior [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Departamento de Física, Química e Biologia / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Instituto Federal de Educação, Ciência e Tecnologia do Triângulo Mineiro; [4] Universidade de São Paulo
Investigations on new reactions using the well-defined catalysts for olefin metathesis and ethylene polymerization have been occurred around the world.1,2 On the other hand, there is a stimulating challenge in the search for simpler systems, in which an active catalytic species could be readily generated in-situ at low cost. In this direction, we have been developing of alternative Ru/Pd-based catalyst, the novel ruthenium-palladium heterobimetallic complex was synthesized in two steps, [Pd(PPh3)(DMSIO)] (1) synthesis, which reacted with [RuCl2(p-cymene)]2 giving the bimetallic [RuCl2(p-cymene)-Pd(PPh3)(DMSIO)] (2). The complex [RuCl2(p-cymene)(isoniazid)] (3) was synthetized according to the literature2 to compare its reactivity with complex 2. The complexes were characterized by FTIR, UV-Vis and 1H, 13C{1H} and 31P{1H} NMR. The complexes 2 and 3 were evaluated as catalytic precursors for ROMP of norbornene (NBE) and the complex 3 has been evaluated for ethylene polymerization. The polynorbornene (polyNBE) syntheses via ROMP using the complexes 2 and 3 as pre-catalysts were evaluated under reaction conditions of [EDA]/[Ru] = 28 (5 mL), [NBE]/[Ru] = 3500 for 60 minutes at 50 °C, both the complexes were active and the yields were

12 and 17 % respectively. The polymerization of ethylene mediated by palladium complex precursor 1 was active using MAO (Methylaluminoxane) as initiator with a [MAO]/[Pd] ratio of 700, then the complex 2 will be evaluated in the same conditions.

Sais de bis-benzimidazólio próticos como organocatalisadores altamente eficientes na cicloadição de CO2 e epóxidos.

https://proceedings.science/p/120610

Werberson de Almeida Bezerra [1]; Rafael Pavão das Chagas [1]
[1] Universidade Federal de Goiás

A series of efficient, inexpensive and easily prepared protic bis-benzimidazolium salts were first investigate as organocatalysts in the cycloaddition of CO2 and epoxides in absence of metal and solve

Síntese de Tiossulfonatos via Oxidação de Tióis com Peróxido de Hidrogênio-ureia e Catálise de Disselenetos

https://proceedings.science/p/120647

Juliano Alex Roehrs [1]; Bruno da Rosa [2]; Rodrigo Kickofel Steinhorst [2]; Bruno Souza [3]; Juliano B. Azeredo [4]; Marcelo Godoi [5]
[1] Instituto Federal de Educação, Ciência e Tecnologia Sul-Rio-Grandense; [2] IFSul; [3] Universidade Federal de Santa Catarina; [4] Universidade Federal do Pampa; [5] Universidade Federal do Rio Grande

• Green synthesis of thiosulfonate.
• Thiol oxidation catalized by 2, 2'-Dipyridyl Diselenide.
• Urea-Hydrogen Peroxide (UHP) as a green oxidant.
Selenium reagent as catalyst

Síntese e caracterização de MCM-41 modificado com estanho para conversão de biomassa

https://proceedings.science/p/120530

Bruna E. B. Costa [1]; Rayanne Ferreira Damasceno [1]; Antonio Osimar Sousa da Silva [1]; Simoni Margareti Plentz Meneghetti [1]
[1] Universidade Federal de Alagoas

Synthesis of SnMCM-41 by the non-hydrothermal method. Unprecedented tin precursor for modifying MCM-41.

Surface acidity study of KSF clay pillared with aluminum oxide pillars

https://proceedings.science/p/120197

Verônica Lima da Silva [1]; Maria Clara Cardoso Tavares [2]; Manuela Lisboa de Oliveira [3]; RONALDO COSTA SANTOS [4]; Luiz Antonio Magalhaes Pontes [5]
[1] Universidade Federal da Bahia (UFBA) ; [2] Departamento de Engenharia / Faculdade / Universidade Salvador (UNIFACS); [3] Universidade Federal da Bahia (UFBA)/ Programa de Pós-Graduação em Engenharia Química (PPEQ); [4] Unijorge; [5] Universidade Federal da Bahia (UFBA)/ Departamento de Engenharia Química

Different applications for montmorillonite clay are explored. Superficial acidity is an important parameter for organic reactions. Pillarization influenced the acidic nature of pillared clay.

Synthesis and characterization of MOFs containing Cu or Zn metal centers for post-synthesis sulfonation.

https://proceedings.science/p/120344

Rayane Cristine Gomes Aciole [1]; Rômulo Pereira de Almeida [1]; Leonis Lourenço da Luz [2]; Severino Alves Júnior [2]; Ivoneide de Carvalho Lopes Barros [1]
[1] UFRPE; [2] UFPE

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Synthesis of Au nanoparticle catalysts in the form of nanospheres and nanorods supported on TiO2

https://proceedings.science/p/119581

Daniell Daywison Cirilo Silva [1]; Pedro Pablo Florez Rodriguez [1]; Aracelis José Pamphile Adrian [1]
[1] Instituto de Química e Biotecnologia, Universidade Federal de Alagoas

Synthesis and characterization of 1 wt% Au/TiO2 catalysts with Au nanospheres and nanorods. Catalysts were prepared by successive impregnation, which could affect Au nanorods morphology.

Synthesis of cobalt and iron catalysts supported on graphitic carbon nitride and evaluation on HMF oxidation to FDCA

https://proceedings.science/p/120600

Sancler Vasconcelos [1]; Joao Pedro Reys de Mattos [1]; Arthur da Cunha Paes Gil Ventura [1]; Vinicius Rossa [1]; Thiago de Melo Lima [1]
[1] Universidade Federal Fluminense

FDCA is an important precursor of green polymers. This study reports the use of inexpensive non-noble metals catalysts such as Co and Fe supported on graphitic carbon nitride (g-C3N4)

Synthesis, characterization and application of photocatalyst Co(x%)-TiO2 by Sol-Gel method with high environmental potential

https://proceedings.science/p/119502

Thais Torres dos Anjos [1]; Marcos de Oliveira Melo [1]; Klebson Souza Santos [1]
[1] Universidade Estadual de Feira de Santana

Synthesis of semiconductor Co(x%)-TiO2 with photodegradation action of cyanide species; Use of the sol-gel method as a route for the synthesis of nanoparticles doped with Co.

The use of a biocatalyst immobilized on magnetic nanoparticles in the conversion of xylose to xylulose

https://proceedings.science/p/119521

João Gabriel Moraes Junqueira [1]
[1] Universidade Federal de São Carlos

For energy production, the world depends to a large extent on non-renewable fossil fuels, mainly in the transport sector1. Therefore, the use of a renewable and sustainable energy source, such as lignocellulosic biomass (sugarcane bagasse and straw, corn stover, among others), it becomes a viable alternative in the second-generation (2G) bioethanol production. The chemical composition of lignocellulosic residues mainly contains cellulose and hemicellulose, which by hydrolysis, produce mostly glucose and xylose, respectively. These monosaccharides can be converted to 2G bioethanol through the alcoholic fermentation carried out by yeasts2. However, the main yeast used in ethanol production, *Saccharomyces cerevisiae*, cannot naturally metabolize xylose. For this reason, the use of new technological routes, such as enzymatic catalysis, becomes an alternative to increase the 2G bioethanol production. In

this context, the enzyme xylose isomerase (XI) that catalyzes the interconversion of xylose to xylulose, a product easily fermented by *S. cerevisiae*, was applied as a heterogeneous biocatalyst, through its immobilization by crosslinking with the glutaraldehyde in Fe3O4 magnetic nanoparticles (MNPs). Fe3O4 MNPs were synthesized by a coprecipitation method3 in the presence of the 1-methyl-3-octadecyl-imidazolium bromide ionic liquid, previously synthesized and characterized, in the chloroform and water mixture. In this way, it was possible to obtain nanoparticles of controlled size, between 2 and 8 nm, which were characterized by transmission electron microscopy (TEM). Some parameters are considered important in the enzyme-support immobilization reaction, because during this process there may be a significant loss of its catalytic activity. For this reason, the immobilization parameters were minutely optimized using 2^6-3 fractional factorial design, which resulted in six independent variables. The response (dependent variable) was the quantification of the reaction product (D-xylulose), after immobilized XI catalytic activity, using a method developed by liquid chromatography coupled to mass spectrometry (LC-MS). The independent variables were: Fe3O4 MNPs, glutaraldehyde, enzyme, pH, temperature, and time. Among them, only the pH showed a greater influence on the immobilization process. The heterogeneous biocatalyst with the highest conversion of D-xylulose obtained from the factorial design was 65%, while the free XI converted 35%. In conclusion, the use of XI immobilized on Fe3O4 MNPs showed a catalytic activation when compared to the use of the free enzyme in solution. **References**: 1. Zabed, H., Sahu, J. N., Boyce, A. N. & Faruq, G. Fuel ethanol production from lignocellulosic biomass: An overview on feedstocks and technological approaches. Renew. Sustain. Energy Rev. 66, 751–774 (2016). 2. Victor, B., Ali, M. & Indati, S. An overview of integration opportunities for sustainable bioethanol production from first- and second-generation sugar-based feedstocks. J. Clean. Prod. 245, 118857 (2020). 3. Laurent, S. et al. Erratum: Magnetic iron oxide nanoparticles: Synthesis, stabilization, vectorization, physicochemical characterizations, and biological applications. Chem. Rev. 110, 2574 (2010).

Tin and niobium oxides applied in fructose conversion: influence of the presence of Lewis and Brønsted acids on catalytic performance

https://proceedings.science/p/119503

Thatiane Veríssimo dos Santos [1]; Dhara Pryston [1]; Geovânia Cordeiro [1]; Mario Roberto Meneghetti [1]; Simoni Margareti Plentz Meneghetti [1]

[1] Universidade Federal de Alagoas, Grupo de catálise e Reatividade Química e Instituto de Química e Biotecnologia.

Fructose conversion was investigated using heterogeneous tin and niobium oxide catalysts in order to obtain chemicals of industrial interest.

TRANSFORMATIONS OF TERPENES AND TERPENOIDS VIA CARBON-CARBON DOUBLE BOND CROSS-METATHESIS

https://proceedings.science/p/120512

Luciana Fernandes [1]; Dalmo Mandelli [1]; Christian Bruneau [2]; Cedric Fischmeister [2]

[1] Universidade Federal do ABC; [2] Université de Rennes 1

Olefin cross-metathesis from sterically demanding natural terpenes.
Preparation of functionalized derivatives of β-pinene, limonene, carvone, and limonene epoxide.

Water Photoeletrocatalysis by monolayer nanosheets of molybdenium dissulfide supported on graphene oxide

https://proceedings.science/p/120068

Leon Diez Starke [1]; Daniel Grassechi [2]

[1] UFRJ; [2] Universidade Federal do Rio de Janeiro

-Hydrothermal synthesis of 2d materials
-Doping transition metal dichalcogenides with transition metals for tunning band-gap
-2d materials heterostrutures

ZSM-5 as a Support for Copper-Based Catalysts for Catalytic Applications

https://proceedings.science/p/120474

Gabriela Maria Maffi [1]; Anderson J. Schwanke [2]; Rosana Balzer [3]

[1] Universidade Estadual do Oeste do Paraná; [2] Universidade Federal do Rio Grande do Sul; [3] Universidade Federal do Paraná – Campus Palotina

Chemical Transformation of R-(+)-limonene. R-(+)-limonene is a natural monocyclic monoterpene of great abundance in Brazil. The ZSM-5 is composed of pentassil units with a Mobil Five type structure.

Eletroquímica e Eletroanalítica - ELE

3D-printed reduced graphene oxide/polylactic acid electrodes: Improved single-step prototyped platform for sensing and biosensing applications

https://proceedings.science/p/120467

Wilson da Silva Fernandes Junior [1]; Vinicius Aparecido Oliani Pedro da Silva [1]; Diego Pessoa Rocha [2]; Jéssica Santos Stefano [3]; Rodrigo Muñoz [2]; Juliano A. Bonacin [4]; Bruno Janegitz [5]

[1] DCNME / Centro de Ciências Agrárias / Universidade Federal de São Carlos; [2] Instituto de Química / Universidade Federal de Uberlândia; [3] Instituto de Química / Universidade Federal de São Carlos; [4] Universidade Estadual de Campinas; [5] Universidade Federal de São Carlos

A new electrochemical system platform using 3D-printing with reduced graphene oxide-doped PLA filament was proposed. The rGO-PLA electrodes were applied for the determination of serotonin and catechol

A Non-enzymatic Ag/δ-FeOOH Sensor for Hydrogen Peroxide Determination using Disposable Carbon-based Electrochemical Cells

https://proceedings.science/p/120519

André Santiago Afonso [1]; Sayton Felipe Resende [1]; Marcio Cesar Pereira [2]; Luiz Henrique Capparelli Mattoso [3]; Ronaldo Farias [4]; Flavio de Meira [1]; Douglas Santos Monteiro [1]

[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Instituto de Ciência, Engenharia e Tecnologia / Universidade Federal dos Vales do Jequitinhonha e Mucuri; [3] Bolsista produtividade CNPq / EMBRAPA; [4] Universidade Federal de São Carlos

A novel non-enzymatic sensor based on δ-FeOOH modified with Ag nanoparticles was fabricated and used to determine H2O2. Ag/δ-FeOOH was synthesized by a simple, reproducible, and fast method.

A platinized Pt microelectrode for sensitive detection of nitric oxide

https://proceedings.science/p/119914

Ana Caroline Belarmino Barros [1]; Douglas Philip Martinez Saraiva [2]; Mauro Bertotti [2]

[1] Instituto de Química da Universidade de São Paulo; [2] Universidade de São Paulo

Nitric oxide is a free radical, gaseous at room temperature, colorless, highly reactive and one of the main mediators of intra and extracellular processes. Endogenously produced nitric oxide has been studied extensively in the past years owing to its roles in numerous physiological processes, which include neurotransmission, vasodilatation, blood pressure regulation, and angiogenesis. In vivo NO measurements are challenging because such compound is present in low concentrations in the body (sub μM levels) and is highly reactive. Thus, the development of sensitive and selective NO electrochemical sensors is an exciting challenge to be faced. Accordingly, in this work we show our efforts to modify the surface of a Pt microelectrode (r = 25 μm) by platinization for further application of such a platform for the anodic oxidation of NO. The platinization was performed at controlled potential in a H2PtCl6 + 0.5 M H2SO4 solution for varying deposition times. The electrochemical oxidation of NO occurs at around 0.7 V (vs. Ag/AgCl) for the bare Pt microelectrode, whereas the roughened electrode surface of the platinized Pt microelectrode enables faster electron-transfer kinetics. As a consequence, a much sharper voltammetric wave is noticed with a remarkable current

enhancement. This is possibly attributed to the formation of metallic surface sites, which facilitate the electron-transfer step, associated with the significant increase in surface area. The enlarged surface is responsible for the increased capacitive current, as readily observed in the voltammograms recorded with the platinized Pt microelectrode. Notwithstanding, in comparison to bare Pt microelectrode, the platinized one showed enhanced sensitivity for NO detection. The influence of some experimental parameters such as deposition potential, deposition time, and H2PtCl6 concentration on the anodic oxidation of NO was systematically investigated.

Altered Electrochemistry of Amiloride Drug on Boron-Doped Diamond Electrode: Studies for Selective Detection in Urine by Square Wave Voltammetry and Application in the Doping Control

https://proceedings.science/p/119784

Karla Aparecida de Oliveira Souza [1]; Ana Mara Fonseca [1]; Dilton Martins Pimentel [1]; Andréa Renata Malagutti [1]; Wallans Torres Pio Santos [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

This work presents a novel electrochemical behavior study of amiloride drug on boron-doped diamond electrode, showing, for the first time, a reduction process for selective detection of this drug.

Analytical determination of azametiphos in Billings water dam using flow injection analysis with amperometric detection

https://proceedings.science/p/120380

Marília de Almeida Maeda [1]; Thays Lima [2]; Tiago Luiz Ferreira [1]; Lucia Codognoto [3]; Fábio Henrique Ferreira Batista [1]
[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo - Campus Diadema; [3] Universidade Federal de São Paulo - Campus de Diadema - SP
Azametiphos (AZT) is a pesticide belonging to the group of organophosphates classified as highly toxic, and recently this active compound was banned in Brazil [1-2]. The aim of this work is the study of the oxidation of AZT on BDD electrode in aqueous media and development an electroanalytical methodology using the BDD electrode as amperometric detector for a flow injection analysis system, for the quantification of the AZT in natural waters. The electrochemical measurements were performed using an AUTOLAB PGSTAT 128N potentiostat/galvanostat, cyclic voltammetry and flow injection analysis along with amperometric detection. The flow injection analysis (FIA) system was composed of a high precision multichannel peristaltic pump from Ismatec with tygon tubes, a proportional injector with a sample loop of 30 µL and an amperometric detector composed of the BDD (5000 ppm) working electrode, Ag/ AgCl (3.0 mol L−1 KCl) reference electrode and platinum wire as auxiliary electrode. The measurements were performed with amperometric detection at the operating potential of 1.7 V, with a flow rate of 30 mL min−1. A stock solution of AZT was prepared in the concentration of 1.0x10-3 mol L-1 in acetonitrile and the other solutions were obtained from dilutions of this solution. AZT showed oxidation peak at 1.7 V, with irreversible process characteristics and controlled by species diffusion. An analytical curve was constructed in the linear range of 1.0x10-5 mol L-1 to 5.0x10-4 mol L-1,(y= [5,8x10-7 + 0,150x] / r=0,999) and the limits of detection and quantification were 3,89x10-8 mol L-1 and 1,29x10-7 mol L-1, respectively. The method was applied to the determination of AZT in waters of the Billings dam (Figure 1A and 1B), and its performance indicate the possibility of determinate AZT in waters collected from the Billings dam in Diadema - SP.

Aspectos fundamentais da interconversão eletroquímica de grupos álcool, carbonila e ácido em Platina

https://proceedings.science/p/120398

Pablo Fernández [1]
[1] Universidade Estadual de Campinas
Electrosynthesis will play an important role in the development of a sustainable bioeconomy. Fundamental studies are mandatory to understand the electrochemical interconversion of organic groups.

Avaliação experimental da atividade anticorrosiva de imino-derivados da 4-cloro-chalcona em aço carbono AISI 1020 em meio ácido

https://proceedings.science/p/119959

Mariana Falcão Lopes Princisval Carlos [1]; Aurea Echevarria [1]
[1] Universidade Federal Rural do Rio de Janeiro

Synthesis and anticorrosion evaluation of enaminoesters halogenated aniline derivatives against steel carbon AISI 1020 in acid medium. This work performed the evaluation of theanti-corrosion effect.

Avaliação gravimétrica de dois inibidores de corrosão verdes para aço doce em meio ácido.

https://proceedings.science/p/120595

Lucas Guedes [1]; Caio Machado Fernandes [2]; Eduardo Ponzio [1]; Leonardo Alvarez [3]
[1] Universidade Federal Fluminense; [2] Instituto de Química / Universidade Federal Fluminense; [3] Universidad da Costa Rica

Environmental-friendly synthesis of two benzylidene derivatives.
Corrosion inhibition activity with average best efficiency of 92% at 4.50 mmol L −1 .

Batch-Injection Amperometric Determination of Tetracycline using a screen-printed electrode decorated with AuNPs

https://proceedings.science/p/119692

Luana Rianne da Rocha [1]; César Tarley [1]
[1] Universidade Estadual de Londrina

New electrochemical method using BIA system for TCs determination.

First development of analytical methods with portable characteristics, favoring in-situ¬ analysis.

Biochar and Graphene derivative in the development of sensitive and selective electrode to carbendazim determination

https://proceedings.science/p/120692

Jonatas de Oliveira Souza Silva [1]; Mércia Vieira da Silva Sant'Anna [2]; Sanny Wedja Melo Machado de Carvalho [1]; Ava Gevaerd [3]; Ewerton Santos [1]; Alberto Wisniewski Jr [4]; Luiz Humberto Marcolino-Jr [5]; Márcio Fernando Bergamini [5]; Eliana Sussuchi [2]
[1] Universidade Federal de Sergipe; [2] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [3] Universidade Federal do Paraná; [4] Universidade Federal de Sergipe, Brasil.; [5] Instituto Federal do Paraná

A modified carbon electrode was developed based on biochar and reduced graphene oxide. The proposed sensor was successfully applied for the determination of CBZ in a spiked whole orange juice sample.

Biomimetic Sensor Applied in the Free Radical Electrochemical Generation from the Nitrofurazone Reduction in Aqueous Media

https://proceedings.science/p/120132

Mauro Aquiles La-Scalea [1]
[1] Universidade Federal de São Paulo

Caracterização do processo de oxidação da isatina-3-tiosemicarbazona

https://proceedings.science/p/120648

Lucas Martins Correa Böhs [1]; Juliano da Rosa Justim [1]; Juliano Justim [1]; Bianca Barreto Martins [2]; Bianca Martins [2]; Ana Paula Lopes de Melo [2]; Ana Paula Lopes de Melo [2]; Katlen Bandeira [2]; Katlen Bandeira [2]; Vanessa Carratú Gervini [2]; Vanessa Gervini [2]; Leandro Bresolin [2]; Marcelo Godoi [1]; Carlos Roberto De Menezes Peixoto [3]

[1] Universidade Federal do Rio Grande, Escola de Química e Alimentos, Campus Santo Antônio da Patrulha.; [2] Universidade Federal do Rio Grande, Escola de Química e Alimentos, Campus Carreiros.; [3] Universidade Federal do Rio Grande/Escola de Química e Alimentos

Isatin-thiosemicarbazone derivatives have relevant pharmacological activity. Oxidation of isatin-thiosemicarbazone derivatives generates isatin and thiourea.

Caracterização eletroquímica do fungicida Boscalida por voltametria cíclica e de onda quadrada

https://proceedings.science/p/120413

Priscila Azevedo Liberato [1]; Astréa Filomena de Souza Silva [2]; Leonardo Luiz Okumura [1]

[1] Centro de Ciências Exatas e Tecnológicas / Departamento de Química / Universidade Federal de Viçosa - Campus Viçosa; [2] Departamento de Química - CCE - Universidade Federal de Viçosa

Electroanalytical study of the fungicide Boscalida by cyclic voltammetry and square wave. Optimization of electroanalytical methodology for determining Boscalida by cyclic voltammetry (CV) and square.

Carbon paste electrode modified with cork as a sensor for the determination of Pb2+

https://proceedings.science/p/120619

Thalita Medeiros Barros [1]; Elisama Vieira dos Santos; Iasmin B. Silva [1]; Carlos Alberto Martínez-Huitle [1]; Mayra Monteiro [1]; Djalma Ribeiro da Silva [1]

[1] Universidade Federal do Rio Grande do Norte

The results showed clearly, cork-graphite sensors, GrRAC presented a linear response with r2 of 0.99 and 0.98, as well as limits of detection and quantification of 0.25 µM and 0.87 µM, respectively.

Chemical deposition of THF and POLY (Phenylene Sulphide Phenylenamine) - PPSA films on iron

https://proceedings.science/p/120070

David Alexandro Graves [1]; Carla Oliveira Pereira da Silva [2]; Andrea Santos Liu [1]; Emerson Sarmento Gonçalves [2]; Liu Yao Cho [3]; Priscila M.S.C.M. Leite [4]

[1] IFSP; [2] ITA; [3] UNIVAP (FEAU e IP&D); [4] UNIVAP

The synthesis of new protective materials from corrosion of metals, as well of metal alloys, has being proven to be one of the most promising research branches, concerning both the scientific importance in understanding this phenomenon and its potential technological applications (SPINKS, 2002). Polyaniline forms a class of conducting polymers, and the emerald state may reach the highest conductivity values. Low synthesis pH can trigger oxidation reactions of the metal, competing with the oxidation of the monomer, hindering the polymerization process and may result in low polymer adhesion on the metal surface (MATTOSO, 1995). In addition, the insolubility of PAni that makes it difficult to deposit this polymer by methods that need the dissolved polymer (VILCA, 2003). Thus, the use of new soluble derivatives of PAni (such as PPSA) has been investigated by numerous research groups (CAMILO, 2006). The objective of this work is the synthesis of a film obtained by the chemical deposition of a solution with THF (BALASKAS, 2011) and PPSA (LEUNINGER, 1998). The methodology involved, thus, 1) the chemical deposition of the film with a micropipette; 2) appraisal procedures by SEM (scanning electron microscope), sequentially in EDX (energy dispersive x-ray detector), what could permit the analysis on the behavior of film (SHINEN, 2015). To evaluate the data, an automatic image detection process was carried out, so that it was possible to evaluate the structures present in the chemically deposited films, allowing the study of the formation of circles and their occurrence. The Hough transform is a standard method for detecting shapes that are easily parameterized (lines, circles, etc) in digitized images, originally designed to detect analytically representable features in binary images, as well as lines and circles (DUDA, 1972). The edges of an image must be detected so that the Hough transform can be applied, for that, a Gaussian filter is applied to better identify the image and eliminate noise, a process of expansion and erosion to highlight the contours and finally a Sobel filter (GILG, 2017), being an operation used for image processing for edge detection, consisting of an operator

that calculates the intensity gradient of an image at each point, showing the direction of the greatest variation from light to dark, thus, it is possible to locate the edges of the image (A) (CONCI, 2009). With the result of the transformation, the center and the radius of the circles were obtained and it was possible to construct a histogram (B) with the identification of the frequency of these rays and their respective sizes, being also possible to verify their replicability.

Copper nanostructured microsensor developed electrochemically for determination of glyphosate in river water samples.

https://proceedings.science/p/119940

Gilberto J. Silva Junior [1]; Daniel Matias Gaston Regiart [2]; Mauro Bertotti [1]
[1] Universidade de São Paulo; [2] Instituto de Quimica - USP

NPC film was electrodeposited on a copper microelectrode and then used for the electrochemical detection of Glyp. The good sensor performance was demonstrated by detection Glyp in river water samples.

Copper oxide gas diffusion electrode for light assisted CO2 reduction

https://proceedings.science/p/119592

Claudia Longo [1]; MIGUEL T. GALANTE [1]; Leonardo A. A. Silva [1]; Natália A. Reis [1]
[1] Instituto de Química-UNICAMP

Methanol was produced from CO2 reduction in 1h electrolysis performed at -0.3 V (vs Ag/AgCl) using Cu2O-Gas Diffusion Electrode irradiated by solar simulator under CO2 flow in NaHCO3 aqueous solution

Desenvolvimento de eletrodos compósitos a base de acrilonitrila-butadieno-estireno (ABS) e grafite modificados com hexacianoferratos metálicos

https://proceedings.science/p/120526

Grasielli Correa de Oliveira [1]; Janiny Lacerda [1]; Ricardo Cassella [1]; Eduardo Ariel Ponzio [1]
[1] Universidade Federal Fluminense

Development of composite electrodes based on ABS and graphite modified with metallic hexacyanoferrates synthesized via sonochemistry for possible applications in electroanalytical determinations.

Desenvolvimento de sensor eletroquímico descartável para detecção de Vitamina B12.

https://proceedings.science/p/120490

Ana Carolina Alves Ananias [1]; Kamylla de Paula Venancio [2]; Lívia Flório Sgobbi [2]
[1] Instituto de Química / Universidade Federal de Goiás; [2] Universidade Federal de Goiás

Detection of vitamin B12 by square wave voltammetry (SWV) in aqueous medium with KCl (0.1M) in pH 3 phosphate plug, using conductive carbon ink electrode manufactured by the screen printing method.

Determination of Lysergic Acid Diethylamide (LSD) by Square Wave Voltammetry using Boron-Doped Diamond Electrode: Electrochemical Screening Method for Seized Samples in Forensics Analysis

https://proceedings.science/p/119889

Luan Mendonça santos [1]; Dilton Martins Pimentel [1]; Luciano Arantes [2]; Wallans Torres Pio Santos [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Polícia Civil do Distrito Federal

We present a simple and fast voltammetric method for determining LSD on absorbent papers using the boron-doped diamond electrode, offering easy on-site analysis and screeninyg of seized samples.

Development of an electrochemical method for direct determination of Mephedrone using a sensor modified with graphene oxide

https://proceedings.science/p/119689

Maiyara Carolyne Prete [1]; César Tarley [1]
[1] Universidade Estadual de Londrina

Only two works report the direct determination of Mephedrone using disposables SPE. The GCE modified with GO is a potential simple and sensitive method for the direct detection of Mephedrone.

Electroanalytical determination of estradiol in Billings waters dam

https://proceedings.science/p/120382

Letícia Torquato Viana [1]; Calixto Fernandes Filho [2]; Thays de Souza Lima [3]; Lucia Codognoto [4]
[1] Universidade Federal de São Paulo - Campus Diadema; [2] Instituto de Ciências Ambientais, Químicas e Farmacêuticas / Universidade Federal de São Paulo - Campus Diadema; [3] Universidade Federal de São Paulo; [4] Universidade Federal de São Paulo - Campus de Diadema - SP
Development an electroanalytical methodology using the BDD electrode for the quantification of the hormone E2 in natural waters. Determination of emerging pollutants in the environment.

Electroanalytical determination of the glycosylated flavonoid Canferitrin in infusions of Bauhinia forficata using diamond electrodes

https://proceedings.science/p/119897

Carolina Godinho Simião [1]; Carolina Zeni Pires Mecca [1]; Eliana Maíra Valle [1]; THIAGO VEIGA [1]; Lucia Codognoto [2]
[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo - Campus de Diadema - SP
Study of the electrochemical behavior of canferitrin on the BDD electrodes. Development of an electroanalytical methodology for the determination of this flavonoid in infusions of Bauhinia forficata.

Electroanalytical study of the interaction between DNA immobilized on magnetic nanoparticles and Polycyclic Aromatic Hydrocarbon

https://proceedings.science/p/120399

Débora Batista Pinheiro Sousa [1]; Antônio Gomes dos Santos Neto [1]; Gilvanda Silva Nunes [1]; Paulo Roberto B. de Oliveira Marques [2]; Raimunda Nonata Fortes Carvalho Neta [1]
[1] Universidade Estadual do Maranhão; [2] Universidade Federal do Maranhão

Detection of electroanalytical DNA signal, Interaction between DNA and polycyclic aromatic compounds, Magnetic nanoparticles immobilization. Printed electrodes .

Electrocatalysis of hydrogen oxidation on platinum decorated nanoporous gold surface using scanning electrochemical microscopy

https://proceedings.science/p/119952

Jéssica Soares Guimaraes Selva [1]; Anandhakumar Sukeri [2]; Mauro Bertotti [1]
[1] Universidade de São Paulo / Instituto de Química, Departamento de Química; [2] Universidade de São Paulo / Instituto de Física de São Carlos, Departamento de Física

A Pt-NPG surface was prepared via anodization method to explore the H2 oxidation electrocatalysis using the feedback mode of SECM. The positive feedback current was observed at the Pt-NPG surface.

ELECTROCHEMICAL DETECTION OF CADMIUM (II) AND LEAD (II) IONS USING GRAPHITE ELECTRODES MODIFIED WITH POLY(P-CUMARIC ACID)

https://proceedings.science/p/120601

Thaís Machado Lima [1]; Diego Leoni Franco; Lucas Franco Ferreira [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Graphite electrodes modified with polymeric films of p-coumaric acid were used to detect lead and cadmium ions in aqueous solutions where concentrations up to 2.0 ppb were monitored.

Electrochemical sensor based activated biochar and reduced oxide graphene to determination of paraquat

https://proceedings.science/p/119443

Mércia Vieira da Silva Sant'Anna [1]; Ava Gevaerd [2]; Jonatas de Oliveira Souza Silva [3]; Lucas dos Santos Lima [3]; Márcio Fernando Bergamini [2]; Eliana Sussuchi [1]
[1] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [2] Universidade Federal do Paraná; [3] Universidade Federal de Sergipe

Activation of the “Aguapé” biochar surface. Use of activated biochar and reduced graphene oxide for the development of electrochemical sensors. Composite electrode sensitive to paraquat detection.

Electrochemical sensor based on protic ionic liquid used in the determination of carbendazim in grape juice

https://proceedings.science/p/119414

José Fernando Macedo [1]; Anderson Alex C. Alves [2]; Mércia Vieira da Silva Sant'Anna [1]; Frederico G. C. Cunha [3]; Eliana Sussuchi [1]
[1] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [2] Universidade Federal de Sergipe (UFS); [3] Departamento de Física (DFI) / Universidade Federal de Sergipe (UFS)

Electrochemical sensor modified with protic ionic liquid showed greater sensitivity. The sensor developed was successfully applied for monitoring carbendazim in grape juice.

Electrochemical sensors based on ionic liquid and reduced graphene oxide for voltammetric determination of ciprofloxacin

https://proceedings.science/p/119441

Michael Douglas Santos Monteiro

Electrochemical study of a clinically applied UHMWPE biomaterial modified with Ti, Zr, and Ta

https://proceedings.science/p/120229

Higor Gomes Quevedo [1]; Melissa Machado Rodrigues [2]; Cristian Padilha Fontoura [2]; Carlos Alejandro Figueroa [2]; Klester dos Santos Souza [1]; Cesar Aguzzoli [2]; Carlos Alejandro Figueroa [2]
[1] Universidade Federal do Rio Grande do Sul; [2] Universidade de Caxias do Sul (UCS)

Alternative material for articulation in total joint replacement improving surface properties of UHMWPE by deposition of Ti, Zr, Ta films Ta-PE presented better passivate and topological properties

Electrochemically reduced graphene oxide films on interdigitated electrodes as field-effect transistors

https://proceedings.science/p/120027

Nirton Cristi Silva Vieira [1]
[1] Universidade Federal de São Paulo

Graphene oxide (GO) is a graphene derivative with oxygen-containing functional groups in its basal plane and its borders. These functional groups facilitate GO dispersion in various solvents, including water, allowing the deposition of this material on numerous kinds of substrates and surfaces. GO contains a mixture of carbon atoms with sp2 and sp3 hybridization, which gives an insulating character to this material [1]. However, the partial reduction of oxygen-containing functional groups produces another derivative of graphene. Reduced graphene oxide (rGO) presents a certain π conjugated structure and consequent electrical conductivity [2]. rGO has been proving to be an excellent alternative to pristine graphene in electronic devices, especially in terms of cost and processability. In this study, GO sheets were deposited onto interdigitated gold electrodes and reduced via cyclic voltammetry (CV) to realize solution-gated field-effect transistors (SG-FETs) [3]. GO reduction was carried out in a conventional electrochemical cell containing the electrolyte and three electrodes: an interdigitated electrode having GO films as a working electrode, Ag/AgCl reference electrode, and a platinum plate as the auxiliary electrode. Electrochemical reduction avoids the use of dangerous reductants agents, high temperatures, and also eliminates byproducts. SG-FETs with high transconductance (over 100 μS) were achieved. In the future, the devices will be applied as sensors for the detection of cyanotoxins. Experiments in this direction are in progress. 1. Dreyer, D.R., et al., The chemistry of graphene oxide. Chemical society reviews, 2010. 39(1): p. 228-240. 2. Pei, S. and H.-M. Cheng, The reduction of graphene oxide. Carbon, 2012. 50(9): p. 3210-3228. 3. Vieira, N., et al., Graphene field-effect transistor array with integrated electrolytic gates scaled to 200 mm. Journal of Physics: Condensed Matter, 2016. 28(8): p. 085302.

Electrodeposition and characterization of Sn-In coatings from a deep eutectic solvent based on choline chloride

https://proceedings.science/p/120521

Natalia Gomes Sousa [1]; Paulo Naftali da Silva Casciano [2]; Pedro de Lima-Neto [3]; Adriana Nunes Correia
[1] UFC- Universidade Federal do Ceará; [2] UNIVERSIDADE FEDERAL DO CEARÁ; [3] Universidade Federal do Ceará

SnIn electrodeposition from deep eutectic solvents based on choline chloride and ethylene glycol. Surfactant acted as a leveling agent, becoming SnIn coatings more homogeneous.

Electrodes based on Aprotic Ionic Liquids for Detection of the Carbendazim

https://proceedings.science/p/119512

Eliana Sussuchi [1]; José Fernando Macedo [1]; José Felipe dos Santos [2]; Mércia Vieira da Silva Sant'Anna [1]; Frederico G. C. Cunha [2]
[1] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [2] Universidade Federal de Sergipe

Ionic liquids with the potential to increase the sensitivity of carbon paste electrodes. Development of sensitive electrodes based on aprotic ionic liquids for the determination of carbendazim.

Electron Lifetime determination by IMVS and EIS to dye sensitized solar cells

https://proceedings.science/p/119813

Gideã Taques Tractz [1]; Danielle Cristina Oliszeski [1]; Everson do Prado Banczek [1]; Maico Taras da Cunha [1]; Paulo Rogerio Pinto Rodrigues [1]
[1] Universidade Estadual do Centro-Oeste

To reduce the use of fossil fuels, solar cells are promissing devices. However understanding the interfacial reactions to produce efficient systems is require and it can be done using electrochemical

Enhanced energy storage of Fe3O4 nanoparticles embedded in N-doped graphene

https://proceedings.science/p/120322

Susana Chauque [1]; Adriano Henrique Braga [1]; Renato V. Gonçalves [2]; Liane Rossi [1]; Roberto M. Torresi [1]
[1] IQ-USP; [2] IFSC - USP

Here, we report the synthesis and application of a hybrid material composed of Fe3O4 nanoparticles embedded in nitrogen-doped graphene sheets (Fe3O4@N-doped graphene) as a negative electrode for lithium-ion batteries. We studied the influence of N-doped graphene on the storage capacity of Fe3O4 using different electrochemical techniques. We determined that the as-prepared Fe3O4 materials presented high-quality crystalline nanostructures. Using cyclic voltammetry and electrochemical impedance spectroscopy techniques, we demonstrated that the N-doped graphene sheets improved the conductivity between the Fe3O4 nanoparticles, allowing a faster charge transfer process than that for pure magnetite nanoparticles, as well as the presence of porous particles in the hybrid composite. The Fe3O4@N-doped graphene hybrid material showed the best Li storage capacity and maintained specific capacity values of 910 mA h g−1 during the first 150 cycles performed at 0.05 A g−1 and 850 mA h g−1 at 0.1 A g−1 during the following 50 cycles, which were near their corresponding theoretical values. Moreover, the N-doped graphene sheets resisted the volume changes that occur during discharge/charge processes, which helped avoid the consequent pulverization that this kind of material suffers in rate capability experiments. We provided a simple and novel method to obtain a material with a higher superficial area and conductivity between particles, allowing great performance as a negative electrode for lithium-ion batteries application.

Estudo comparativo do processo de eletrodeposição de Fe-Co a partir de banhos de eletrodeposição à base de citrato e EDTA

https://proceedings.science/p/120295

William Feitosa de Araújo [1]; Elton Patrick Barbano [2]; Francisco Michel [1]; Mayke Marques Vidal [2]; Thaini Cavalcante Marinho [2]
[1] Universidade Estadual Vale do Acaraú; [2] Universidade Estadual Vale do Acaraú

O interesse pela eletrodeposição de ligas de ferro e cobalto têm aumentado consideravelmente nos últimos anos, principalmente devido às diversas propriedades físicas e químicas relacionadas a essas ligas. Ligas de Fe-Co exibem boa resistência à corrosão, boas propriedades mecânicas e magnéticas. O objetivo do presente trabalho foi realizar um estudo comparativo do processo voltamétrico de deposição de Fe-Co a partir de banhos contendo citrato e ácido etilenodiamino tetra-acético (EDTA) como agentes complexantes para os íons metálicos em solução. Para os estudos voltamétricos foram utilizados uma célula eletroquímica do tipo metrohm para três eletrodos, eletrodo de carbono vítreo como eletrodo de trabalho (ET), Ag/AgCl 3,0 mol/L como eletrodo de referência e uma espiral de platina como eletrodo auxiliar. Para o voltamograma cíclico do substrato de carbono vítreo para o sistema FeCo/citrato (pH 4,0) observou-se um processo catódico c (-0,95 a -1,10 V) e processos anódicos ax (- 0,70 a + 0,05 V). O processo catódico c está relacionado com a codeposição de Fe-Co, visto que o voltamograma da solução “branco” não apresentou processos catódicos e os voltamogramas dos metais individuais Fe-citrato e Co-citrato apresentaram um processo catódico entre 1,00 a 1,10V e 1,10 a 1,25V respectivamente. Para o sistema Fe-Co/EDTA, o voltamograma do ET na solução de trabalho não apresentou picos de deposição, mostrando um significativo aumento na densidade de corrente a partir de -1,10 V siando de 0,5 mA cm-2 para 16 mA cm-2. Comportamento semelhante é observado para os metais individuais, sistemas Fe-EDTA e Co-EDTA, entretanto, por inspeção visual, foi verificado eletrodepósito na superfície do eletrodo (a partir de -1,00 V) para ambos os sistemas e para FeCo/EDTA. Os resultados mostram que há uma diferença significativa no processo de eletrodeposição de Fe-Co quando comparados os complexantes utilizados, com variações nos voltamogramas cíclicos. Ademais é possível verificar que para o sistema Fe-Co/citrato a utilização do complexante foi benéfica deslocando o potencial de deposição da liga para valores mais positivos quando comparado aos metais individuais.

Estudo da ação inibidora da biomassa da microalga Chlorella sorokiniana na corrosão do aço carbono 1020 em meio de HCl 1 mol L-1

https://proceedings.science/p/120608

Gustavo Oliveira [1]; Anita Do Vale [1]; Eliane D'Elia [1]
[1] Universidade Federal do Rio de Janeiro

The microalgae *Chlorella sorokiniana* was studied as a natural corrosion inhibitor through gravimetric and electrochemical tests.

Estudo de diferentes métodos de deposição de Pt sobre filmes finos de Sb2Se3 e seu impacto na fotoatividade catalítica.

https://proceedings.science/p/120579

Marcos Vinicius De Lima Tinoco [1]; Magno Barcelos Costa [2]; Lúcia Mascaro [2]; Juliana Brito [1]
[1] Universidade Federal de São Carlos; [2] Departamento de Química / Universidade Federal de São Carlos

Development of photoelectrochemical catalyst for water splitting; Pt nanoparticles deposition by photocatalysis, electrocatalysis and photoelectrocatalysis; Optical and physical characterization.

Estudo voltamétrico do processo de eletrodeposição de Co-Ni a partir de um banho não cianetado

https://proceedings.science/p/120062

Bruna Maria Rodrigues Gonçalves [1]; Elton Patrick Barbano [2]
[1] Universidade Estadual Vale do Acarau; [2] Universidade Estadual Vale do Acaraú

Voltammetric study of the Co-Ni electrodeposition process from a non-cyanide bath
Voltammetric study of Co-Ni electrodeposition revealed a cathodic process and crack-free coatings Co-Ni binary alloy

Evaluation of complex formation between 5-nitrothiophene-thiosemibazonic derivatives with β-cyclodextrin free and chemically linked to the glassy carbon electrode.

https://proceedings.science/p/119819

Renata Costa dos Santos [1]; Fabricia da Rocha Ferreira [1]; Thiago Mendonça de Aquino [1]; Fabiane Caxico de Abreu [1]
[1] UFAL

The planning and development of new therapeutic agents, nitroheterocyclic compounds are of great importance, enabling the introduction of various substituent radicals, which gives the compounds different activities and properties, both chemical and biological. Its bioreduction mechanism can be reproduced in electroanalytical cells and identified via electrochemical methods. A characteristic common to many nitrocomposites (such as those under study) is the low solubility in water, which justifies its association with versatile substances such as cyclodextrin, which can form inclusion complexes with a variety of molecules1. In the present study, an amino β-cyclodextrin graft was performed on glassy carbon electrodes, through the amine electrooxidation, without the need for additional ligands or intermediates2; then, the formation of inclusion complexes between 5-nitrothiophene-thiosemibazonic derivatives (LNN) and β-cyclodextrin was evaluated using Differential Pulse Voltammetry (VPD). The electrochemical system was composed of 3 electrodes, Ag / AgCl / Cl-saturated (reference), platinum (auxiliary), glassy carbon (CV) with immobilized β-cyclodextrin amino (work), in buffered medium pH 7.00 with ethanol as co-solvent. UV-Vis studies were also carried out in an aqueous medium containing 5% –ethanol, varying the concentration of β-Cyclodextrin. The CV-amino-β-cyclodextrin platform made it possible to analyze the interaction of 5-nitrothiophene-thiosemibazonic derivatives with β-CD, which was identified by linearly increasing the peak current of the analyte as a function of the increase in the concentration of the same until the saturation point between the substances and the β-CD immobilized on the electrode surface and it was possible to calculate the equilibrium constant between the studied derivatives and the cyclodextrin with values from 5,87x104 L.mol-1 for LNN01, 2,199x105 L.mol-1 for LNN03 and 7,61x105 L.mol-1 for LNN05. By spectrophotometric methods, the calculated average constants were 2,107x105 L.mol-1 for LNN01, 2,174x106 L.mol-1 for LNN03 and 2,223x105 L.mol-1 . Both constants demonstrate good formation of the complexes among the LNN: β-CD. Cyclodextrin is already considered a pharmaceutical excipient, used in drugs, so its good results via electrochemistry with the studied derivatives are quite hopeful in a future association and development of a drug

Experimental and theoretical evaluation of 4-chloro-N-(pyridine-2-ylmethyl) aniline as corrosion inhibitor for mild steel in acid media.

https://proceedings.science/p/119988

Caio Machado Fernandes [1]; Marcos Vinicius Palmeira Mello [2]; Nazir dos Santos [3]; Alessandra Mendonça Teles de Souza [4]; Mauricio Lanznaster [3]; Eduardo Ponzio [3]
[1] Instituto de Química / Universidade Federal Fluminense; [2] Universidade Federal Fluminense / Instituto de Química; [3] Universidade Federal Fluminense; [4] Universidade Federal do Rio de Janeiro

Simple and inexpensive synthesis of 4-chloro-N-(pyridine-2-ylmethyl) aniline
Maximum anticorrosive efficiency of 96% at 4.59 mmol/L
Experimental studies, surface analyses and theoretical calculations

Fabrication of disposable laser-scribed electrochemical sensor for detection of picric acid explosive

https://proceedings.science/p/119791

Lillia Iamar Leite Maciel Gama [1]; William Reis de Araujo [1]
[1] UNICAMP

Os explosivos são utilizados com o intuito de cometer crimes, como explodir caixas eletrônicos, cofres de bancos e para auxilio em fugas de presos dos sistemas prisionais, logo, a área forense necessita de métodos que proporcione análises em campo para rápida identificação de amostras suspeitas em locais de crimes1. O uso de técnicas eletroquímicas vem ganhando grande destaque nos últimos anos para o desenvolvimento de métodos rápidos, portáteis e de baixo custo para a detecção de diferentes compostos, como drogas, infecções bacterianas, poluentes, etc. Assim, esses dispositivos portáteis são importantes ferramentas analíticas para identificar materiais suspeitos e/ou detritos diretamente em locais de pós-explosão, e para o monitoramento de locais contaminados (durante etapas de remediação ambiental). Assim, o presente trabalho demonstra a fabricação de sensores eletroquímicos portáteis sobre placas de fenolite utilizando carbonização superficial induzida por radiação de laser de CO22 para a detecção do ácido pícrico, um nitro explosivo de uso militar com fórmula molecular C6H2(OH)(NO2)3 e nomenclatura oficial IUPAC 2,4,6-trinitrofenol, que é sensível ao choque mecânico e a temperaturas elevadas3. Os sensores desenvolvidos foram devidamente caracterizados visando compreender a estrutura e morfologia do material carbonoso formado por meio das técnicas de Microscopia Eletrônica de Varredura (SEM), espectroscopia Raman e eletroquímica (voltametrias e espectroscopia de impedância eletroquímica). Após a otimização dos parâmetros de fabricação, potência do laser, velocidade de varredura e distância focal, a resistência elétrica das trilhas de carbono foi tipicamente de 20 Ωcm-1. Este baixo valor de resistência elétrica associada à sua estrutura porosa identificada por SEM permite alto desempenho nas analises eletroquímicas. A detecção do ácido pícrico foi realizada por meio da técnica de voltametria de onda quadrada utilizando uma faixa de potencial de -0,1 V a -1,0 V. A curva analítica construída em meio de tampão fosfato 0,1 mol L-1 (pH = 2,0) apresentou boa linearidade (R2 = 0,996) entre os valores de pico de corrente com os valores de concentrações na faixa de 5 a 60 µmol L-1 e uma sensibilidade de 0,40 A.L.mol-1. O limite de detecção (LD) e quantificação (LQ) foram calculados utilizando LD = 3σ/S e LQ = 10 σ/S e obtivemos os valores de 9,43E-7 e 3,14E-6, respectivamente. Com base nos resultados podemos concluir que os sensores desenvolvidos são uma excelente proposta para a detecção de ácido pícrico, pois, apresenta baixo custo de fabricação sem a necessidade de reagentes adicionais ou etapas laboriosas, proporcionando ótimas propriedades eletroquímicas, fácil utilização e alta reprodutibilidade. 1 P. Rabenecker and K. Pinkwart, Propellants, Explos. Pyrotech., 2009, 34, 274–279. 2 L. F. Mendes, A. de Siervo, W. Reis de Araujo and T. R. Longo Cesar Paixão, Carbon N. Y., 2020, 159, 110–118. 3 M. Abrel, Tese Mestr., 2006, 1–114.

Fast and Simple Determination of Quinidine in Pharmaceutical Samples by Square Wave Voltammetry Using a Boron-Doped Diamond Electrode

https://proceedings.science/p/120139

Débora Aparecida Rocha Moreira [1]; Dilton Martins Pimentel [2]; Wallans Torres Pio Santos [2]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri ; [2] Universidade Federal dos Vales do Jequitinhonha e Mucuri

The drug Quinidine is an antiarrhythmic agent, which is also used in the treatment of malaria. Quinidine belongs a class of the narrow therapeutic index drugs and its dosage needs to be efficiently controlled. The official method for quinidine determination is based on high performance liquid chromatography with ultraviolet detection. Electrochemical methods have been widely reported for drugs determination in formulations pharmaceutical due to their advantages, such as low-cost, fast and simplicity for the application in the quality control of drugs. In this context, we present, for the first time, an electrochemical sensor for quinidine determination using a boron-doped diamond (BDD) electrode with square wave voltammetry (SQW) detection. Electrochemical measurements were performed on an Autolab PGSTAT 128N potentiostat/galvanostat. Electrochemical cell was composed of three electrodes: BDD with a doping level of 8000 ppm ((0.13 cm2), Ag/AgCl (saturated KCl) and platinum wire as working, reference and auxiliary electrodes, respectively. The BDD electrode was pretreated cathodically in 0.5 mol L−1 H2SO4, applying a current of +0.001 A for 120 s and then applying −0.03 A for 360 s. This treatment of the BDD electrode was performed before each analysis. The electrochemical behavior of quinidine was evaluated by cyclic voltammetry in different pHs and electrolytes. The best condition for quinidine electrochemical detection was obtained using a 0.25 mol L-1 sulfuric acid

solution as electrolyte support, where quinidine showed two irreversible oxidation processes at +0.7 and +1.6 V (vs Ag/AgCl) on BDD. The generated product of quinidine oxidation at 1.62 V presented a reduction process at +0.3 V on DDB. The mass transport of quinidine was investigated and the oxidation process is controlled by diffusion at BDD. The second oxidation process of quinidine at BDD (1.6 V vs Ag/AgCl) is more sensitive for detection and quantification of this drug. However, the reduction process generated by second anodic peak of quinidine was selected to determine this drug due to its more selectivity for detection in pharmaceutical samples. Thereby, before the quinidine detection by SWV using BDD electrode, the application of an oxidation potential and its duration time were optimized at +1.7 V and 90 s, respectively. The parameters of the SWV technique were optimized with amplitude of 90 mV, step of 8 mV and frequency of 60 Hz. In these conditions, the repeatability for determination of 100 µmol L-1 quinidine was performed with a low relative standard deviation of 1.5% (N = 8). Two linear ranges were obtained to quantify quinidine, from 0.2 to 5.2 µmol L-1 and 10.3 to 55.0 µmol L-1, both with linear regression coefficients more than 0.99. The limit of detection (LOD) was calculated to be 0.03 µmol L-1 and the addition-recovery studies in pharmaceutical samples containing quinidine were around 100 %. Therefore, the proposed method has been shown to be promising for a simple, fast and selective analysis of quinidine drug. Furthermore, the use of an unmodified electrode as BDD can be an interesting alternative for the quality control of drugs with lower cost and waste generation than the official methods.

Hybrid palladium-ceria nanorods electrocatalysts for ethanol oxidation reaction

https://proceedings.science/p/119690

Victor dos Santos Pinheiro [1]; Felipe de Moura Souza [1]; Tuani Carla Gentil [1]; Aline Nakagawa do Nascimento [1]; Luanna Silveira Parreira [1]; Mirela Sairre [1]; Bruno Lemos [1]; Mauro Coelho dos Santos [1]
[1] Universidade Federal do ABC

The electrocatalysts with Pd and CeO2 NR showed the highest electrochemically active surface area, mass activity, cell potential, maximum current and power densities in ADEFC experiments.

Influence of different sulfur encapsulation ways in MOFs applied in Li-S batteries

https://proceedings.science/p/119790

Breno Luiz de Souza [1]; Suana Chauque [1]; Paulo Filho Marques de Oliveira [1]; Roberto Manuel Torresi [1]
[1] Universidade de São Paulo

The concerns about the depletion of fossil fuels, global warming caused by the increase of greenhouse gases like CO2, have increased at last years. The science focus consists on the development of new technologies to renew the energy matrix, using renewable energy to decrease the problems. One way is the increase of specific capacity of energy storage materials, specifically the positive electrode (sulfur) in Lithium-Sulfur Batteries (Li-S). The advantages of sulfur as positive electrode are its high theoretical specific capacity (1675 mA h g-1), low cost and abundance. On the other hand its low electric conductivity, shuttle effect caused by dissolution of the discharge/charge intermediates (polysulfides, PS) in organic electrolytes and the volumetric expansion are the challenges to be overcome. The sulfur encapsulation in ZIF8 - zeolitic imidazole framework consist in a good alternative since this kind of MOF are well known as a class of porous materials that can offer diverse geometries and exceptionally high surface area; therefore, they are widely used in the storage, separation and release of guest molecules [1]. Then the sulfur is confined to the ZIF8 pores where charge/discharge processes will take place, avoiding the shuttle and volumetric expansion effects. Here, we report a green synthesis method of ZIF8 by mechanochemistry following by the encapsulation of S8 via different ways to optimize the best condition: (i) By a new synthetic method “one plot”; (ii) physical mixing and (iii) sulfur-melting. The different phase purities were confirmed by XRD, and the morphologies and sulfur distribution by TEM/EDS. The sulfur amount into the MOF was confirmed by TGA curves and the specific capacities were determined considering this sulfur mass. The cyclic voltammetry shows the stability of the composite, where the two reduction peaks are referred to the lithiation process by PS formation and the oxidation peak consists to the PS return to the elemental sulfur form. It was observed that melting incorporation is the best way to incorporate sulfur, showing a especific capacity of 700 mA h g-1. This works shows that MOFs are good approaches to applied in Li-S batteries. [1] ZHENG, Y. et al., Journal of Materials Chemistry A, 7 (2019) 3469-3491

Initial studies of the voltammetric process of electrodeposition of Ni-Mo from a non-cyanide bath

https://proceedings.science/p/119980

Francisco Michel [1]; Mayke Marques Vidal [1]; Elton Patrick Barbano [1]; William Feitosa de Araújo [1]; Thaini Cavalcante Marinho [1]

[1] Universidade Estadual Vale do Acaraú

Initial studies of the voltammetric process of electrodeposition of Ni-Mo from a non-cyanide bath
Voltammetric study of Ni-Mo electrodeposition revealed a cathodic process (-0,80 a -0,92 V) and the us

Interação entre molécula relativamente hidrofílica e copolímeros triblocos monitorado por técnicas eletroquímicas: uma nova abordagem

https://proceedings.science/p/120415

Fernando Rodrigues de Carvalho [1]; Rafael da Silva [1]

[1] Universidade Estadual de Maringá

Electrochemical techniques are very feasible for investigating the interaction effects between electroactive molecules and polymeric micelles systems, providing wide varied of additional information.

Morphology's influence on Pd-based electrocatalysts activity for green fuels oxidation reactions

https://proceedings.science/p/119713

Tuani Carla Gentil [1]; Victor dos Santos Pinheiro [1]; Felipe de Moura Souza [1]; Mauro Coelho dos Santos [1]

[1] Universidade Federal do ABC

Differentiated morphologies such as Pd nanodendrites can favor ethanol oxidation reaction (EOR) in green electrocatalysis processes, allowing to obtain mass activity greater.

NaNbO3 microcubes decorated with Pd as a promising electrocatalyst for ethanol oxidation reaction

https://proceedings.science/p/120014

Felipe de Moura Souza [1]; Victor dos Santos Pinheiro [1]; Tuani Carla Gentil [1]; Luanna Silveira Parreira [1]; Bruno Lemos [2]; Mauro Coelho dos Santos

[1] Universidade Federal do ABC; [2] UFABC

Sodium niobate microcubes decorated by Pd nanoparticles are 6 times more electrocatalytically active for Ethanol Oxidation Reaction (EOR) than the commercial material Pd/C Alfa Aesar (AA).

Oxidação eletroquímica de Fention em água da Represa Billings

https://proceedings.science/p/120604

Thays de Souza Lima [1]; Lucia Codognoto [2]; Diogo Oliveira Silva [3]; Fábio Ruiz Simões ; Eliana Maíra Valle [1]; Heron Dominguez Torres da Silva [4]; Gustavo Barbosa dos Reis [1]; Cristiane Santana [1]; Mauro Coelho dos Santos [5]

[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo - Campus de Diadema - SP; [3] Universidade Federal de São Paulo - Campus Diadema; [4] Universidade Federal de São Paulo - Campus Baixada Santista; [5] Universidade Federal do ABC

The electrolysis was monitored using SWV, UV-Visible absorption spectrometry and liquid chromatography with mass detector (LC-MS). The decay of the FEN signal was observed during electrolysis.

Photoelectrochemical properties under ultraviolet light of a metal-organic framework structure based on cobalt obtained by precipitation synthesis

https://proceedings.science/p/119989

Luiz Henrique Dallantonia [1]; Paulo Rogerio Catarini da Silva [2]; Adriana Campano Lucilha [2]; Luan Pereira Camargo [2]
[1] Departamento de Química / Centro de Ciências Exatas / Universidade Estadual de Londrina; [2] Universidade Estadual de Londrina

MOF-Co was easily synthetized by the precipitation method.
It presents very good electrochemical properties showing a high photocurrent under UV light.

Preliminary Evaluation of Polypyrrole Electrosynthesis on Structural Carbon Fibers for Energy Storage and Transmission

https://proceedings.science/p/119734

Lucas Vaz [1]
[1] Instituto Federal de Educação, Ciência e Tecnologia de São Paulo

Conducting polymers have several properties that make them useful as aerospace materials, including low density, moderate cost, excellent corrosion resistance and high conductivity. Due to its high intrinsic conductivity, thermal stability, high energy density, as well as its viability in synthetic approaches, Polypyrrole (PPy) was one of the most studied polymer-based conductive electrode materials for batteries and supercapacitors.In this work, a light flexible electrode composed of PPy electrodeposited on a carbon fiber surface was obtained electrochemically using an efficient one-step procedure, through a galvanostatic method. All the Polypyrrole in this work was obtained by electrosynthesis in structural carbon fiber. PPy deposition was performed by electrosynthesis in a three electrode cell from 0.1 molL-1 of freshly distilled pyrrole solution with 0.5 molL-1 sulfuric acid.The working electrode for the deposition of PPy was a 5 cm "smooth" Hexcel 282-50 GRAPHITE carbon fiber cable with 3000 filaments of 7.1 µm in diameter.The electrodes were morphologically characterized by Scanning Electron Microscopy. The composition and structure of the electrodes were characterized by Raman, FTIR and XRD. In addition, the capacitive performance of the electrodes was investigated by Cyclic Voltammetry; Galvanostatic Charge-Discharge and Electrochemical Impedance Spectroscopy, performed with in the potential window of -0.2 to 1.2V (vs. Ag / AgCl) in electrolyte 1.0 mol.L-1 of H2SO4, as a scan rate at 10mV.s-1 . Therefore, it was found that the carbon fiber material coated with PPy exhibited much more pronounced electroactivity than the pure carbon fiber electrode, including excellent fiber-polymer interaction. As shown in Figure 1, the CV curves of the PPy electrode, compared to the carbon fiber not coated with PPy, indicate its highly capacitive behavior. As shown in Figure 2, the growth morphology of PPy on carbon fiber is represented by a very thin film on its surface and between monofilaments, composed of numerous agglomerated and tiny nanoparticles that form a relatively dense structure. As shown in Figure 3, the high frequency EIS of the pure carbon fiber electrode exhibits greater resistance to charge transfer compared to the PPy electrode [9]. In addition, the greatest resistance related to the material at low frequencies is that of the pure carbon fiber electrode. These significant improvements in the electrochemical properties of the PPy electrode can be attributed to its improved conductivity due to the conductive carbon fiber substrate and the electrode and electrolyte contact, in addition to its porous structure and large surface area.

Sensor eletroquímico baseado em líquido iônico e óxido de grafeno reduzido para determinação voltamétrica de ciprofloxacina

https://proceedings.science/p/119415

Michael Douglas Santos Monteiro [1]; Mércia Vieira da Silva Sant'Anna [2]; Anderson Alex C. Alves [3]; José Fernando Macedo [2]; Eliana Sussuchi [2]
[1] Universidade Federal de Sergipe; [2] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [3] Universidade Federal de Sergipe (UFS)

The novel sensor electrochemical of modified carbon paste electrode with reduced graphene oxide and ionic liquid for detection ciprofloxacin. The proposed method presented LOD = 4.21 nmol L-1.

Síntese de Co3O4 a partir da reciclagem de baterias de íon-Li exauridas e sua aplicação como pseudocapacitor

https://proceedings.science/p/120495

Edson Lucas Dosval Coelho [1]; Fernando Silva Betim [1]; Sandra Aparecida Duarte Ferreira [1]; Maria de Fátima Fontes Lelis [1]; Marcos Freitas [1]

[1] Universidade Federal do Espírito Santo

Recycling spent Li-ion batteries
Synthesis of Co3O4
Application as an electrochemical pseudocapacitor

Studies for simple and fast determination of hydrochlorothiazide in pharmaceutical samples and urine using boron-doped diamond electrode

https://proceedings.science/p/119908

Larissa Magalhães de Almeida Melo [1]; Fernando de Jesus Souza [1]; Anne Alves Macedo [1]; Dilton Martins Pimentel [1]; Wallans Torres Pio Santos [1]

[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Hydrochlorothiazide (HCTZ) is a drug with diuretic action, which its use is mainly associated with the treatment of arterial hypertension and it can also be used in other types of treatment, such as congestive heart failure, liver cirrhosis and others. HCTZ is banned by the World Anti-Doping Agency (WADA)1. This because, in recent years, this drug has been used by athletes in sports competitions of different modalities for the purpose of weight-loss and/or to disguise the use of other prohibited substances by WADA. Due to this the quality-control of this drugs in pharmaceutical formulation is very important, as well as in urine sample is interest to WADA. The Several analytical methods have been used for drugs detection in quality control and anti-doping analysis, but most notably chromatographic methods with UV and mass spectrometry detection. Nevertheless, electroanalytical methods can offer easy on-site screening method of samples, providing a portable, simple and low-cost electrochemical sensors. In this context, we present the HCTZ determination using an unmodified electrode of boron-doped diamond (BDD) as electrochemical sensor. The BBD electrode was used with square wave voltammetry (SWV) technique was used for a fast and sensitive detection of HCTZ in urine and its possible application as a screening method in the doping control. The measurements were carried out in an electrochemical cell with three electrodes, using BDD as the working electrode (with doping of 8.000 ppm and an area of 0.13 cm^2) and Ag/AgCl (saturated KCl) and platinum wires as reference and auxiliary electrodes, respectively. The BDD electrode was pretreated cathodically and anodically in 0.5 mol L−1 H2SO4: for the cathodic pretreatment, first was applied a positive current of +0.001 A for 120 s and then applied −0.03 A for 360 s; for the anodic pretreatment was applied the same currents above, but first was applied the negative current. The two pretreatments of BDD electrode were evaluated and the cathodic treatment was chosen, which was performed before each analysis. The HCTZ electrochemical behavior was studied by cyclic voltammetry (CV) in Britton-Robson buffer (BRB) solutions (pH 2 to 12) and other electrolytes. The best conditions in function to higher sensitivity and a better selectivity for HCTZ detection were obtained in 0.1 mol L^{-1} BRB pH 2.0 at BDD electrode, where an oxidation process for HCTZ at +1.3V was observed. The repeatability of SWV and differential pulse voltammetry (DPV) techniques were evaluated for a reproducibible and sensitive detection of HCTZ. The relative standard deviations of 2.6% and 6.5% were obtained for 10 determination of 1 mmol L-1 HCTZ by SWV and DPV, respectively. Thereby, SWV technique was chosen to determinate of this analyte with all parameters previous optimized: potential step of 5 mV, amplitude of 80 mV and frequency of 40 Hz. Linear range for HCTZ quantification was obtained from 0.8 to 6.9 µmol L-1 (r2=0.999) with low LOD of 0.2 µmol L-1. The addition-recovery studies in pharmaceutical samples containing HCTZ were obtained around 100 %. The interference study in urine samples are being performed. Therefore, proposed method offers a fast and simple alternative for the quality control of HCTZ. Furthermore, due to good sensitive achieved using the BDD electrode with SWV detection, this sensor presents a perspective to be a screening method for doping control analysis of HCTZ in urine samples.

Study of inhibitory efficiency of ethanol and Goji Berry extract on corrosion of SAE 1045 carbon steel

https://proceedings.science/p/119815

Danielle Cristina Oliszeski [1]; Gideã Taques Tractz [1]; Danielle Borges [1]; Everson do Prado Banczek [1]; Maico Taras da Cunha [1]; Paulo Rogerio Pinto Rodrigues [1]

[1] Universidade Estadual do Centro-Oeste

Goji Berry extract can be used as a green corrosion inhibitor. In this study the efficiency was 89% against corrosion of carbon steel, due to the synergistic effect with ethanol.

Study on the application of thin films of MnO2/Au nanoparticles as an H2O2 amperometric sensor

https://proceedings.science/p/119967

Vítor Mendes Miguel [1]; Maria Paula de Souza Rodriges [1]; Susana Inês Córdoba Torresi

[1] Universidade de São Paulo

The determination of H2O2 concentration is extremely important in environmental, food, industrial and pharmaceutical sectors, and the construction of sensors capable of carrying out this determination with precision and efficiency has been extensively studied over the years. Among the methods of determination, the electrochemical methods stand out for the simplicity and analysis speed, being developed several sensors based on materials capable of reacting catalytically with H2O2. MnO2 nanoparticles have a great catalytic activity in the decomposition of H2O2 and have been used for the manufacture of several sensors using different methods of film deposition. Its application in conjunction with other metals, in particular Au, shows very promising results for combining catalytic properties of the two materials, thus increasing the catalytic current generated in the decomposition of H2O2. In this work, thin films of MnO2 nanowires decorated with Au nanoparticles were deposited on ITO glass electrodes using a drop casting method. Calibrations curves were constructed using a amperometric method by aplying a potential of 0,6 V with or without visible light (523 nm) irradiation. The results obtained with the material decorated or not with Au were studied showing great improves in the sensibility of the sensor with the adition of gold due to photoelectrochemical and plasmonic effects.

Synthesis and characterization of a Fe-based cathode for lithium-ion batteries.

https://proceedings.science/p/120559

Helder Rezende de Oliveira Filho [1]; Nickolas Victor Barbosa Caldas [1]; Pei San E [2]; John Low [2]; Sukarno Olavo Ferreira [1]; Robson S. Monteiro [3]; Reinaldo Teófilo [1]

[1] Universidade Federal de Viçosa; [2] University of Warwick; [3] Catalysis Consultoria Ltda.

Synthesis of layered cathode LiFeCoMnO2 for lithium batteries was performed. The materials were synthesized with high purity. Mixture design was applied to define the compositions of the materials.

The effect of EDTA on the morphological characteristics of the copper-tin electrodeposits.

https://proceedings.science/p/120221

Elton Patrick Barbano [1]; Mayke Marques Vidal [1]; Francisco Michel [1]; Thaini Cavalcante Marinho [1]; William Feitosa de Araújo [1]

[1] Universidade Estadual Vale do Acaraú

The voltammetric studies showed that the EDTA complexing agent had a beneficial effect. SEM analysis of deposits showed that 1010 steel electrode was totally covered by a deposit and crystallites.

The effect of tin addition to platinum nanoparticles catalysts with different morphologies towards methanol electrooxidation reaction in alkaline media

https://proceedings.science/p/120464

Rebecca dos Anjos [1]; Aíla dos Santos [2]; Rodolfo Antoniassi [3]; Odivaldo Alves [1]; Júlio César Martins Silva [1]
[1] Universidade Federal Fluminense; [2] Instituto de Química / Universidade Federal Fluminense; [3] Universidade de São Paulo

Pt/C and PtSnO2/C cubic nanoparticles with preferential Pt(100) orientation; The effect of tin addition to platinum towards methanol electrooxidation in alkaline media; High catalytic activity.

The influence of stepped Pt[n(111)×(110)] electrodes towards glycerol electrooxidation: Electrochemical and FTIR studies

https://proceedings.science/p/120195

Vinicius Del Colle [1]; Camilo A. Angelucci; Luiza Maria da Silva Nunes; Germano Tremiliosi Filho
[1] Universidade Federal de Alagoas

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Tin electrodeposition on platinum substrates from ionic liquid and deep eutectic solvent: a comparative study

https://proceedings.science/p/120145

João Francisco Sousa Salgueira [1]; Ana Aline Coêlho Alcanfor [1]; Adriana Nunes Correia [1]; Pedro de Lima-Neto [1]; Giancarlo Richard Salazar Banda [2]; Katlin Ivon Barrios Eguiluz [2]
[1] Universidade Federal do Ceará; [2] Universidade Tiradentes

Tin electrodeposition from 1-butyl-3-methylimidazolium chloride and from 1ChCl:2EG. Catalytic effect for the Sn2+ reduction process at 23.5 and 80.0 oC.

Tuning the synthesis of ZrO2 into Printex L6 carbon by hydrothermal method assisted by microwave oven: an improve of the activity for H2O2 electrogeneration

https://proceedings.science/p/120144

Matheus Schiavon Kro 2017/23464-3) [1]; Guilherme Fortunato [1]; Paulo Cordeiro-Júnior [1]; Marcos Lanza [1]
[1] Instituto de Química de São Carlos (IQSC-USP)

Optimization of hydrothermal synthesis of ZrO2 into carbon black by microwave-assisted method using short time reaction and low temperature. Shift of ~140 mV the onset ORR keeping the high selectivity

Use of cyclic voltammetry for antioxidant capacity determination of Cunila angustifolia BENTH extract

https://proceedings.science/p/120267

Diulia Chananeco Fofonka [1]; Matheus Henrique Oliveira de Sousa [1]; Neusa Moura [2]; Carlos Roberto de Menezes Peixoto [2]
[1] Universidade Federal do Rio Grande; [2] Universidade Federal do Rio Grande/Escola de Química e Alimentos

Electrochemical methods are very efficient and simple for total antioxidant capacity determination.
Cunila angustifolia BENTH is a plant with high antioxidant potential.

Use of recycled silver in the modification of composite electrodes for analytical applications
https://proceedings.science/p/119809

Taíssa da Silva Cabral [1]; Suellen Fabricia Lima do Nascimento [1]; Rafael Dornellas [1]; Wagner Pacheco [1]
[1] Universidade Federal Fluminense
The silver extracted from photo residues was used to modify the surface of composite electrodes in the form of a film or nanoparticles, in order to obtain improvements in their performance.

Ensino de Química - EDU

"What is the reaction?": a game proposal to discuss named organic reactions
https://proceedings.science/p/120079

Ricardo Lima Guimarães [1]; Arantcha Lorran Nardi [1]; Arthur Neves [1]; Nayalle Raíssa da Silva Batista [1]
[1] Universidade Federal de Pernambuco - UFPE

Proposal for the elaboration of a didactic game to discuss named organic reactions for undergraduate chemistry classes. The game is expected to promote the recognition and identification of these reactions.

A FORMAÇÃO DE PROFESSORES DE QUÍMICA NOS INSTITUTOS FEDERAIS: EDUCAÇÃO AMBIENTAL EM PERSPECTIVA
https://proceedings.science/p/119726

Nyuara Araújo da Silva Mesquita [1]
[1] UFG

A mobilização de saberes docentes por licencia(n)dos em Química no contexto de visitas a museus
https://proceedings.science/p/120051

Camila Silveira Silva [1]; Maryna Bringmann [1]; Aline Kundlatsch [1]
[1] Universidade Federal do Paraná
The mobilization of teaching knowledge by undergraduate students and teacher Chemistry in the context of visits to museums: visits to museums provided the mobilization of teaching knowledge in its four dimensions, in addition to allowing a cultural, scientific and integrative approach, revealing aspects that allow understanding educational processes the museums in conjunction with teacher training.

A TEACHING SEQUENCE FOR THE STUDY OF SOLUTIONS IN HIGH SCHOOL
https://proceedings.science/p/119586

Carlos Cezar da Silva [1]; Alexandre Fermanian Neto [1]
[1] Instituto Federal de Educação, Ciência e Tecnologia de Goiás
A Sequência Didática (SD) foi elaborada numa abordagem em Ciência, Tecnologia e Sociedade (CTS)1 para o estudo de soluções, baseou-se na experiência dos pesquisadores que observam excesso de conteúdo na segunda série do ensino médio, além do obstáculo que o professor geralmente encontra durante a contextualização de soluções. A SD foi construída a partir de um levantamento de conhecimentos anteriores, abordando os temas “tratamento de água e soluções químicas”, apresentação de vídeos sobre o tema. A aplicação de um questionário contendo questões dissertativas serviu como indicação do conhecimento dos alunos sobre o assunto2, visita a uma estação de tratamento de água, atividade no laboratório envolvendo análise de amostras de água, e, posteriormente, um questionário após as

atividades que continha questões dissertativas sobre o assunto abordado3. Participaram desta pesquisa 25 alunos de uma escola pública na cidade de Barra do Garças, estado de Mato Grosso, Brasil. O Questionário final continha as seguintes indagações: 1- Quais as etapas para o tratamento da água e as substâncias químicas utilizadas em cada etapa?; 2- Diferencie: água natural e tratada; 3- Como podemos definir soluções?; 4- Você acha que é possível calcular a quantidade (concentração) de substâncias químicas presentes na água?, Se sua resposta for SIM, teria uma ideia de como calcular essa concentração?; 5 - O que é uma água dura?; 6- Diferencie: titulante e titulado.; 7- O que é uma titulação química? Os resultados das questões foram organizados no Gráfico 1, a seguir. Gráfico 1: Análise do questionário pós-sequência didática. Fonte: Arquivo pessoal dos pesquisadores (2019) A sequência didática desenvolvida para o ensino de soluções químicas, proporcionou aos educandos melhorar seus conhecimentos e contribuiu para contornar as dificuldades encontradas nos temas abordados no processo de obtenção, classificação e tratamento de água para consumo humano, além da análise de parâmetros físico-químicos. 1SANTOS, W. L. P.; AULER, D. (Org.) CTS e educação científica: desafios, tendências e resultados de pesquisas. Brasília:Ed. Universidade de Brasília, 2011. 2MORAES, R.; GALIAZZI, M. C. Análise textual: discursiva. 3. ed. Revisada e Ampliada. Ijuí: Editora Unijuí, 2016. 3 MENEZES, J.C.S. et al. Abordagem do conteúdo soluções com enfoque CTS no ensino de Química: O caso do rio Sergipe no Brasil. In. CONGRESSO IBERO-AMERICANO DE CIÊNCIA, TECNOLOGIA, INOVAÇÃO E EDUCAÇÃO. Buenos Aires, Argentina, 2014. Disponível em: <http://www.oei.es/congreso2014/memoriactei/1514.pdf>. Acesso em: 08 Fev. 2020. Agradecimentos: Instituto Federal de Educação, Ciência e Tecnologia de Goiás, Câmpus Jataí. Programa de Pós-Graduação em Educação para Ciências e Matemática (PPGECM).

A trajetória de alunos da EJA profissionalizante do IFG – Uma análise da relação com o saber

https://proceedings.science/p/120496

Brenda Souza Bento [1]; Gabriel Amorim Vilela [1]; Ramon Marcelino Ribeiro Júnior [1]; Agustina Rosa Echeverría [1]
[1] Universidade Federal de Goiás

- The meaning of learning was identified by a memory reconstitution interview.
- Resolution of drug calculation exercises identified the effectiveness of the study activity.

A utilização dos Três Momentos Pedagógicos de Demétrio Delizoicov no Ensino de Fissão e Fusão Nuclear.

https://proceedings.science/p/119432

Gabriela Fernanda Pinto da Silva [1]
[1] UFPA

Adaptação do jogo ludo para o ensino de termoquímica

https://proceedings.science/p/120288

Juliana Siqueira Duarte [1]; Arielly Celestino Rodrigues Santos [2]; Carmem Adriana da Silva [3]; Elane Elane Chavero Soares [1]
[1] Universidade Federal do Mato Grosso; [2] Universidade Federal de Mato Grosso (UFMT); [3] SEDUC/MT- Secretaria de Educação
Atualmente o jogo didático tem ganhado espaço como instrumento estimulante no processo de aprendizagem nos conhecimentos de química1, à medida que novas atividades são propostas aos estudantes. Os jogos didáticos possuem funções lúdica e educativas, exercem fascínio em crianças e adultos2, exercitando o raciocínio, despertando o interesse e a motivação necessários para uma melhor assimilação do conteúdo abordado3. Nesse sentido este trabalho teve por objetivo analisar a aplicabilidade do jogo Ludo, como instrumento facilitador na compreensão e revisão de conceitos sobre o conteúdo de termoquímica4, analisando ainda o desempenho dos estudantes após a aplicação do jogo. O jogo possui baixo custo e de fácil confecção. O mesmo foi reelaborado e adaptado para ser aplicado junto aos estudantes do segundo ano do ensino médio. Os materiais utilizados para a confecção do jogo foram: Papel cartão, tesoura, peões (de outros jogos) e dados. O jogo permite dois, três ou quatro jogadores (no caso de quatro, é possível formar duas duplas). À medida que o jogo vai se desenrolando, o estudante pode retirar cartas como “ajuda” que o professor ou outro material disposto pode auxiliar na questão ou cartões com questões numéricas onde o jogador deve apresentar o cálculo para avançar no jogo. Durante a partida o estudante tem contato com cartas

e pontos no tabuleiro que o incentivam a entender como é a ação da energia nos processos endotérmico e exotérmico. A atividade proposta surtiu ótimos resultados, os alunos se sentiram incentivados a levantar pontos relevantes, participaram de discussões pertinentes quanto á classificação dos tipos de energia, bem como dos cálculos desenvolvidos durante as aulas. Todavia, ressaltamos que os alunos já contavam com os conceitos prévios necessários ao entendimento das definições relacionadas à Termoquímica, e alguns conseguiram detectar ideias errôneas, confirmando assim o sucesso do uso deste e outros materiais lúdicos no ensino de química. Referências 1MATIAS, S.F. et al. Rev de Pesquisa Interdisciplinar. 2017. 2MAFRA, C.R.S, et al. Programa de Desenvolvimento Educacional. 2009 3KARPINSKI, A.C, et al. Cadernos PDE, vol 1. 2013. 4BATISTA, G.F, et al. 4° Simpósio Nordestino de Química. 2018

Análise da estrutura conceitual do tema interações intermoleculares presente em um livro didático de Ensino Superior.

https://proceedings.science/p/120646

Flavio Antonio Maximiano [1]; João Messias Jr [2]
[1] Instituto de Química USP; [2] Universidade de São Paulo

We use complex network metrics to study the conceptual structure on the topic of intermolecular forces present in a textbook. We also identified the facts, concepts, and principles about this theme.

Análise de Similares de Jogos Educativos e Digitais para o Ensino de Química

https://proceedings.science/p/120063

Tiago Soares Silva [1]; Adriana Vieira dos Santos [2]
[1] Instituto Federal da Bahia campus Santo Amaro; [2] Instituto Federal da Bahia campus Lauro de Freitas

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Application of principal component analysis as part of an instrumental analysis course for undergraduate students

https://proceedings.science/p/120611

Laryssa Santos [1]; Humberto Novaes [1]; Vinicius Montalvão [1]; Paula Fernandes de Aguiar [1]
[1] Universidade Federal do Rio de Janeiro

A lesson script was proposed, in which it introduces some concepts of the statistical tool Principal Component Analysis in a chemistry course for undergraduate students.

As Funções do Jogo Pedagógico no Ensino de Química

https://proceedings.science/p/120019

Thiago Cardoso de Deus [1]; Márlon H.F.B Soares [2]
[1] Instituto Federal de Goiás; [2] Universidade Federal de Goiás

A utilização de jogos pedagógicos no ensino de química deve levar em conta aspectos que permitam o aparecimento de características como a liberdade, voluntariedade, autonomia, curiosidade, discussão entre os pares e com o professor, diagnóstico, imersão do jogador e o jogo social, com regras explicitas e implícitas. O jogo Pedagógico, ou seja, aquele utilizado em um ambiente formal de aprendizagem, deve apresentar um equilíbrio entre a função lúdica do jogo, ligada ao divertimento e a função educativa, ligada ao aprendizado. Assim, jogar em sala de aula se torna prazeroso, uma atividade livre e voluntária, que avalia e ensina o aluno. Pensar o jogo pedagógico requer atenção a cinco funções do jogo que, quando equilibradas, permitem uma maior imersão dos jogadores, a avaliação dos conhecimentos existentes, a estruturação da personalidade e da capacidade de convívio social e o aprendizado. Neste sentido, apresentamos cinco funções do jogo pedagógico presentes em todos os tipos de jogos e que, quando equilibradas, podem potencializar a diversão (função lúdica) e o aprendizado (função educativa) dos alunos. A Função Educativa Formativa se caracteriza pela discussão conceitual que o jogo pedagógico proporciona. A discussão conceitual permite a aprendizagem colaborativa e cooperativa. A Função Educativa Avaliativa se caracteriza pela

capacidade do jogo em avaliar o conhecimento dos alunos acerca dos conceitos e procedimentos de laboratório. Um diagnóstico importante para prática pedagógica. A Função Lúdica Imersiva se caracteriza pela capacidade do jogo em promover a imersão do jogador. Quanto mais imerso no jogo, mais livremente o jogador discutirá os conceitos objetivados. A Função Lúdica Moral se caracteriza pela capacidade do jogo em fazer com que os jogadores entendam as regras do jogo e as utilizem para o bem-estar coletivo. Entender, seguir e modificar as regras do jogo caracteriza os jogadores como iguais e cria laços sociais afetivos. A Função de Equilíbrio do Professor se caracteriza pela capacidade do professor em, ao propor eu utilizar um jogo pedagógico, observar a presença das outras funções e realizar adequações sempre que houver disparidade entre elas.

AS POSSIBILIDADES E FRAGILIDADES DO TRABALHO COM PROJETOS NO ESTÁGIO DA LICENCIATURA EM QUÍMICA DO IF GOIANO

https://proceedings.science/p/119526

Adrielly Aparecida de Oliveira [1]; Rosenilde Nogueira Paniago [2]
[1] Universidade Federal do Triângulo Mineiro; [2] Instituto Federal de Educação, Ciência e Tecnologia Goiano

Brazilian chemistry undergraduate students: An analysis of the socioeconomic profile based on Enade reports

https://proceedings.science/p/120347

Priscila Micaelly da Silva Costa [1]; Rachel Azevedo Maia [2]; Ana Araújo [1]; Mayra Nascimento [1]; Paulo Geglio [2]; Dayse das Neves Moreira [2]
[1] Universidade Federal da Paraíba – Campus Areia; [2] Universidade Federal da Paraíba

Enade Area Report as an important database. Profile of undergraduate chemistry students. Student questionnaire analysis.

Can women be scientists? Engaging girls in STEM in Southern Brazil

https://proceedings.science/p/119887

Marta Regina dos Santos Nunes [1]; Priscilla Mena Zamberlan [1]; Bruna Fisher [1]; Ketlin Worm [1]; Laura Lopes [2]; Tassia Silva [1]; Viven Lopes [1]
[1] Universidade Estadual do Rio Grande do Sul; [2] Uniasselvi

Nowdays, 50% of the available vacancies in Brazilian Public Universities are reserved - quotas law- for students from public high school students, low-income families, colored (black and brown), and native people. According to government statistics, the enrollment of colored students has had a significant increment. Today, black students represent more than 50% of the undergraduate enrollments. However, only 12% of black and brown women are in STEM courses, such as Engineers and Mathematics. About 35% are enrolled in social science, administration, and law, followed by 24% in education. This scenario is similar in the US, despite the country's long-term programs to increase women's participation in these fields. The percentage of African American women is only 13.02% in STEM in the USA. It shows asymmetries between men and women in the sciences are a transcultural phenomenon. Studies on intersectionality draw attention to the importance of multiple stereotypes related to student's cross-identities and their impact on the professional achievements of black women in general. Other studies showed that Elementary School is the better place/time to stimulated girls to study Science and Math. The goal of this paper is to present the results of the project called “Girls in Science” that was developed in 2019 at Santa Cruz do Sul, in the Southern state of Rio Grande do Sul, Brazil with the purpose to address these asymmetries. The Project developed school practices and didactic experiments on Natural Science with girls students (12 to 15 years) and also includes discussion about gender bias and race. The activities were coordinated by Professors and graduate students from the Bioprocess e Biotechnology Engineer course of Universidade Estadual do Rio Grande do Sul for nine months. We used different strategies to teach experimental activities in the Biology and Chemistry fields: movies, experiments in the laboratory, and lectures. At the end of the project, participants shown significant interest in sciences and a better self-trust in running experiments. We evaluate their perception about the nature of the professional work on Natural Sciences has not only improved but also becomes a personal alternative for their own future.

Case Study in Chemistry Teaching: a review in Sociedade Brasileira de Química journals

https://proceedings.science/p/119703

Flávia Maggioni Bernardi [1]; Maurícius Selvero Pazinato [1]
[1] Universidade Federal do Rio Grande do Sul

Literature review about Case Study method in Sociedade Brasileira de Química journals about the last ten years. Twenty articles were identified that seek the developing of an active teaching

Concepções prévias de alunos do 6° ano do ensino fundamental sobre plásticos e microplásticos

https://proceedings.science/p/119905

Rosemary Rodrigues de Oliveira [1]; Tiago Fabricio Carabolante [1]; Luciana Maria Saran [2]
[1] Universidade Estadual Paulista (UNESP), Faculdade de Ciências Agrárias e Veterinárias (FCAV); [2] Universidade Estadual Paulista (UNESP), Faculdade de Ciências Agrárias e Veterinárias (FCAV), Departamento de Tecnologia (DT)

Os microplásticos, assim como objetos de plástico, de maior tamanho, não são incorporados ao ambiente, visto que são constituídos por polímeros sintéticos, dificilmente degradados nas condições ambientais. A problemática ambiental faz parte do dia a dia dos estudantes, contudo, para que uma atitude crítica perante esses problemas seja desenvolvida faz-se necessária uma educação científica e tecnológica que promova reflexão a respeito do uso e descarte dos plásticos no cotidiano. É consenso na literatura que as concepções que os estudantes possuem são ponto de partida para a construção de novos conhecimentos. Nesse sentido, com o intuito de fornecer subsídios para o desenvolvimento de metodologias de ensino capazes de possibilitar a evolução conceitual a respeito de plásticos e microplásticos dos indivíduos envolvidos no processo de ensino-aprendizagem, foi realizado um levantamento de concepções prévias (LCP) em relação aos plásticos e microplásticos, junto a 73 estudantes do 6° ano do Ensino Fundamental de uma escola estadual do município de Jaboticabal (SP) aplicando-se questionário com 6 perguntas dissertativas. No presente trabalho, é apresentada apenas a análise das respostas dadas pelos alunos para as questões 5 (“O que você sabe sobre microplásticos?”) e 6 (“O que acontece com os lixos de materiais plásticos, como os canudinhos de refrigerante, quando são jogados no mar?”). Os dados foram avaliados por análise de conteúdo. A maioria dos respondentes (58 alunos) não sabe o que são microplásticos (Fig. 1A). Os demais estabelecem relação entre a palavra “microplástico” e “plásticos pequenos” ou “menores” (Fig. 1A), contudo inferimos que estes sujeitos não possuem dimensão microscópica disso que referem como “pequeno”. Para a questão 6 os estudantes se referem ao plástico ainda em sua forma observável (macroplástico) (Fig. 1B). Nenhum aluno se referiu ao microplástico resultante da degradação de resíduos como canudinhos e sacolas plásticas (Fig. 1B). A palavra poluição é citada pela quase totalidade de alunos, contudo não é possível, pelo teor das respostas, inferirmos que os estudantes não possuem o conceito de poluição, apenas reconhecem os efeitos de agentes poluentes. **Fig. 1.** Resultados e análise das questões 5 (A) e 6 (B) do levantamento de concepções prévias. Os resultados evidenciam as lacunas conceituais existentes no aprendizado dos alunos, principalmente o que se refere à dificuldade dos estudantes em conceituarem poluição e de estabelecerem relação entre o potencial do plástico para a poluição e seu tempo de degradação. Sugerem ainda a necessidade de ações em espaços de ensino que promovam uma aprendizagem significativa dos conceitos de poluição, plástico e microplástico. Para tanto, advogamos por metodologias de ensino numa perspectiva CTSA (Ciência, Tecnologia, Sociedade e Ambiente) utilizando estratégias em educação ambiental, visando discussão a respeito de alternativas, como a substituição dos plásticos convencionais pelos biodegradáveis e adoção de medidas de sustentabilidade (redução, reutilização, reciclagem e substituição de objetos de plástico por outros menos nocivos ao ambiente). Com a compreensão desses conceitos e a incorporação dessas atitudes, há a possibilidade da diminuição da poluição e da interferência do homem em ambientes naturais.

Conceptions of a Professor of the USP course of Chemistry concerning “being a Chemistry Teacher”

https://proceedings.science/p/120645

Kauê Gonçalves dos Santos Lira [1]; Caian Cremasco Receputi [2]; Thaiara Magro Pereira [1]; Daisy de Brito Rezende [1]
[1] Universidade de São Paulo; [2] Programa de Pós-Graduação Interunidades em Ensino de Ciências da USP

We present Institute of Chemistry Faculty member´s conceptions about what should be a Chemistry teacher, using data gathered with Oral History and Theory of Social Representations approaches.

Development of a low cost fluorescence platform for didactic applications
https://proceedings.science/p/120105

Tiago Andrade Chimenez [1]; Eric Carvalho Amaral [1]; Agatha Maria Wiatek [1]
[1] Instituto Federal Catarinense
A lab-made platform was built to allow fluorescence intensity measurements of oil and biodiesel samples. The developed platform provides fluorescence intensity results in consonance with literature data. Our Arduino low cost system can be used for didactic purposes as an alternative to commercial spectrofluorimeters.

Dynamic Periodic Table as a pedagogical alternative in Chemistry Teaching
https://proceedings.science/p/119909

Carolina Godinho Simião [1]; Carolina Zeni Pires Mecca [1]; Eliana Maíra Valle [2]; Lucia Codognoto [3]
[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo ; [3] Universidade Federal de São Paulo - Campus de Diadema - SP
A pedagogical alternative for the first contact with chemistry in basic education, using visual and interactive memory aimed at inclusion for children with difficulties in memorization and learning.

Educação para todos: construção de materiais adaptados para alunos com paralisia cerebral
https://proceedings.science/p/119553

Maria Lucia T. Guerra de Mendonça

Elaboração e aplicação do jogo Perfil Periódico como estratégia facilitadora para o aprendizado de Química e para favorecer a interação entre os alunos
https://proceedings.science/p/120407

Beatriz Gatti [1]
[1] Universidade Federal de Juiz de Fora
Shows how the methodology used and living together in the classroom directly influences the learning process. Through a card game, this Project brings didatic games as an importante tool in teaching.

Ensino de Química e as Relações Étnico-Raciais: Uma análise de Sequências de Ensino elaboradas por professores em formação
https://proceedings.science/p/119870

Deysiane Alves Lima dos Santos [1]; Wilmo Ernesto Francisco Junior [1]
[1] Universidade Federal de Alagoas

Considering the requirements posed by law 10.639 / 03, this work aims to expand the discussion of the ethnic-racial issue in Chemistry Teaching through the development of Teaching Sequences.

Ensino de Química Orgânica: Uma Analise dos Aplicativos Disponíveis no " App Store".
https://proceedings.science/p/120334

Diana Cardoso Silva [1]; Vânia Maria Teixeira Carneiro [2]; Vinícius Viana Marto [2]; Fabiana Cristina Lopes [2]
[1] Universidade Federal de Viçosa - Campus Florestal; [2] Universidade Federal de Viçosa - Campus Viçosa

Organic Chemistry Education: an analysis of applications available in "App Store".
Analysis and investigation of applications that address Organic Chemistry content, technical and educational aspects.

EsteQuiz: um jogo para o ensino de estequiometria

https://proceedings.science/p/120643

José Ribeiro Gregório [1]; Rochele da Silva Fernandes [1]
[1] Universidade Federal do Rio Grande do Sul

EsteQuiz is a free didactic game on Stoichiometry for Android, composed by five levels with increasing degrees of difficulty. When fully completed, it supplies a conceptual map on Stoichiometry.

Estratégias didáticas no uso de recursos didáticos digitais para o ensino de Química a partir da aprendizagem tecnológica ativa

https://proceedings.science/p/119719

Sebastião Silva Neto [1]; Bruna Rafaela Ferreira da Silva [1]; Larissa Santos Galvão [1]; Bruno Silva Leite [1]
[1] Universidade Federal Rural de Pernambuco

We propose three didactic strategies in the use of Digital Didactic Resources for Teaching Chemistry based on Active Technological Learning.

Formação Docente Indígena e as Ciências da Natureza: revisando a literatura

https://proceedings.science/p/120491

Eduarda Boing Pinheiro [1]; Fernanda Luiza de Faria [2]
[1] Universidade Federal de Santa Catarina - Campus Blumenau; [2] Departamento de Ciências Exatas e Educação / Centro Tecnológico, de Ciências Exatas e Educação / Universidade Federal de Santa Catarina - Campus Blumenau

State of the art of works related to the training of indigenous teachers in natural sciences;
Interculturality in indigenous schools resists the supremacy of science;
Only three works were found.

From Woman to Woman: narratives about the influence of Marie Curie in my academic and citizen formation.

https://proceedings.science/p/120209

Amanda de Almeida Oliveira [1]; Marcos de Oliveira Melo [2]; Klebson Souza Santos [1]
[1] Departamento de Exatas / Universidade Estadual de Feira de Santana; [2] Universidade Estadual de Feira de Santana

The perspective and vision of women in science; autobiographical notes as an instrument of democratization of the act of thinking and talking about science.

Impressões dos estudantes às aulas remotas de Química durante a pandemia do COVID-19: análise inicial.

https://proceedings.science/p/120494

José Antonio Maruyama [1]; Silvio Henrique Fiscarelli [2]; Eduardo Jesus Tavares [2]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Faculdade de Ciências e Letras / Universidade Estadual Paulista "Júlio de Mesquita Filho"

Remote teaching has become a reality for some students and learning through this methodology is a challenge. Understanding the students' behavior in face of this reality was the challenge of this work

Innovation and chemistry: a (under)graduate course

https://proceedings.science/p/120361

João Bosco Paraiso da Silva [1]; Andre Galembeck [1]

[1] UFPE

Innovation and chemistry is a course that aims to promote innovation as part of the formation of both graduate and undergraduate students.

Jogo análogo ao x0091cara a carax0092 na revisão de conteúdos de Química Orgânica

https://proceedings.science/p/119549

Ana Beatriz Silva Vellosa [1]; Rodrigo Alves de Souza [2]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Secretaria da Educação do Estado de São Paulo

Elaboration and application of a board game similar to 'face to face', to evaluation and review of the content of Organic Chemistry of the 3rd year (technical course integrated to the High School)

Lei n. 10.639/2003: produção da cachaça, uma tecnologia de matriz africana

https://proceedings.science/p/120098

Antonio Cesar Batista Alvino [1]; Antonio Cesar Batista Alvino [1]; Juvan P. da Silva [2]; Marilene B. Moreira [2]; Anna M. C. Benite [2]

[1] Universidade Federal de Goiás; [2] UFG

Highlights Law n. 10.639/2003: production of cachaça, an African technology. The objective of this work was to insert Law n. 10,639 / 2003, in Chemistry Teaching. Cachaça was fermented and distilled for the first time by Africans enslaved in Colonial Brazil. 30 high school students, aged between 13 and 20 years old participated in the research. Resumo/Abstract O objetivo deste trabalho foi inserir no Ensino de Química a Lei n. 10.639/2003, que determina obrigatoriedade do ensino de história e cultura africana e afro-brasileira nas instituições de ensino do Brasil. Para atingir tal objetivo, foi planejado uma Intervenção Pedagógica sobre produção e destilação da cachaça[1]. Participaram da pesquisa 30 estudantes do Ensino Médio, com idade entre 13 e 20 anos. A cachaça foi fermentada e destilado pela primeira vez por africanos escravizados no Brasil Colônia. Os escravizados produziam a cachaça partir da fermentação da cagaça, uma solução açucarada que sobrava após a cristalização do açúcar[2]. Para produzir a cachaça utilizamos um litro de caldo de cana, em seguida foi adicionado as leveduras ao caldo, que fermentou durante 48 horas, após esse período obteve-se uma mistura de sólido e líquido. O líquido foi transferido para um balão de fundo redondo e acoplado ao sistema de destilação (figura 1). Figura 1: destilação da cachaça e resultados. Foram destilado 80 mL divididos em três frações denominadas de cabeça (5 mL), coração (70 mL) e cauda (5 mL).[2] Na fração coração os/as alunos/as fizeram testes para detectar a presença de álcool no destilado. Eles/elas utilizaram uma solução de dicromato de potássio (K2Cr2O7) para identificar a presença de álcool no destilado. O teste foi positivo para álcool, uma vez que os educandos observaram (figura 1) uma mudança na coloração da solução de K2Cr2O7, evidenciando a oxidação do álcool e a redução do íon cromo Cr6+ a Cr3+. Esses resultados possibilitaram discutir reações redox, processos de fermentação e destilação. Agradecimentos/Acknowledgments Agradecemos a Capes e Cnpq por fomentar nossa pesquisa. [1]Souza, L. M. de, Alcarde, A. R.; Lima,F. V. de, Bortoletto, A. M. Produção de cachaça de qualidade... [et al.] . -- Piracicaba: ESALQ, 2013 72 p. : il. [2]PAULO C. D., PEREIRA, L. G., SANCHES, M. B. SANTIN. J. C., SANCHES, S. Produção de cachaça artesanal com cepas de leveduras selvagens. Nativa. 2016.

Limitations presented by the usage of virtual environment tools during remote classes and their impacts over the process of chemistry language acquisition

https://proceedings.science/p/120626

Bruno Yokoo Dionisio [1]; Thelma Fabra Vieira Yokoo Dionisio [2]; Ana Valéria Santos de Lourenço [1]

[1] Universidade Federal de São Paulo; [2] Outros

This paper's objective is to check if currently available resources in remote teaching virtual tools are enough for a proper utilization of chemistry language in chemistry teaching.

Motivos para se estudar temas de relevância científica e social à luz da Teoria Histórico-Cultural: focalizando a Radiação Ionizante

https://proceedings.science/p/120589

Gabriel Tanja de Andrade Silva [1]; Victor Henrique Barbosa Marques [1]; Eder Junio dos Santos Machado [1]; Pedro Henrique Borges Guimarães [1]; Alessandro Costa da Silva [1]; Agustina Rosa Echeverría [1]
[1] Universidade Federal de Goiás

Show how themes about ionizing radiation can help to increase the interest about Science.
Exemplify how important historical cultural theory is for science teaching.

Multi Jogos Tabela Periódica - ferramenta para ensino lúdico tornando a aula divertida e atrativa

https://proceedings.science/p/119571

Ana Maria Pires [1]; Marcos Hirata Kobori [2]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Kobtron

Multi Games Periodic Table - tool for ludic teaching making the class fun and attractive.
How to use in chemistry classes, domino and "set of three" card game.
The real learn by playing.

Multiple Approaches to Intelligence: elaboration of letters as a tool in the Teaching of the History of Chemistry

https://proceedings.science/p/119945

Késia Filadélfia Dionizio Silva Ramos [1]
[1] UFAL

O PROFESSOR SUPERVISOR DO PIBID: CONTRIBUIÇÕES NO DESENVOLVIMENTO PROFISSIONAL DOCENTE

https://proceedings.science/p/120534

Mara Aparecida Alves da Silva [1]; José Gilberto da Silva [2]; Lucas dos Santos Galiza [1]
[1] Universidade Federal do Recôncavo da Bahia; [2] Centro de Formação de Professores / Universidade Federal do Recôncavo da Bahia

Supervisors teachers play a key role in PIBID in organizing and improving the work of fellows.

O uso da "Horta na Escola" e ensino por investigação como ferramentas de ensino e aprendizagem em Bioquímica/Química de Alimentos

https://proceedings.science/p/120435

Maiara Ingrid Cavalcante Queiroz [1]; André Gustavo Ribeiro Mendonça [1]; Ana Catarina Rezende Leite [2]
[1] Universidade Federal de Alagoas; [2] UFAL

Biochemistry/Food Chemistry is a school subject related not interesting by most of students. This subject was performed with investigative questions and the school garden as a practice tool.

O uso do Instagram como facilitador no processo de ensino da Química levando em consideração os conhecimentos prévios dos discentes.

https://proceedings.science/p/119597

Vivianne Galvão Martins [1]; Mauro Braga França [2]; [1]
[1] Instituto Nacional de Tecnologia / INT / DIQAN; [2] Colégio Pedro II

The objective of the present work is to evaluate the use of the Instagram tool in chemistry teaching, through a methodology that privileges the perceptions and previous knowledge of the students of a third grade class of a public school in the state of Rio de Janeiro. The results presented suggest that the use of the Instagram tool can be a facilitator in the teaching and learning process, as long as it is associated with a perspective that takes into account the student's reality.

Oficina de Design Thinking (DT) na formação inicial de professores de química numa perspectiva transformadora e transdisciplinar

https://proceedings.science/p/120577

Ivina Langsdorff Santana [1]; Luciana do Nascimento Rodrigues [1]; Paulo Rogerio Garcez de Moura [1]
[1] Universidade Federal do Espírito Santo, Brazil

This work aims to develops skills using DT and green chemistry to solve artisanal ceramic pot production problems, in transformative and transdisciplinar way, for undergraduate chemistry students.

Orientação na Pós-Graduação: uma revisão bibliográfica

https://proceedings.science/p/119998

Caian Cremasco Receputi [1]; Rodrigo Mota Santos [2]; Vicente Sarubbi Júnior [3]; Daisy de Brito Rezende [4]
[1] Programa de Pós-Graduação Interunidades em Ensino de Ciências da USP; [2] Programa de Pós-Graduação Interunidades em Ensino de Ciências; [3] Curso de Medicina da Universidade Estadual do Mato Grosso do Sul; [4] Instituto de Química da Universidade de São Paulo

Graduate Surpevisor relationship: a Bibliographic Review. In 17 papers that focused on models of orientation we could identify have been identified various categories related to the mentioned relationship.

Perceptions about the influence of the elaboration and application of educational games in the formation of undergraduate chemistry at the UFC.

https://proceedings.science/p/119737

Alessandro Freitas Barbosa [1]; Luiz Henrique da Costa Souza [1]; Francisco Audísio Dias Filho [1]
[1] UFC (Universidade Federal do Ceará)

This work made it possibleto assess the importance of educational games. The students evaluated positively the participation in the development and elaboration stages of the game.

Playful culture as a precursor of pedagogical games in the chemistry teaching

https://proceedings.science/p/119524

Márlon Herbert F. B. Soares [1]; Nyuara A. S. Mesquita [1]
[1] UNIVERSIDADE FEDERAL DE GOIÁS

Considerando-se o aumento expressivo do uso de jogos pedagógicos no ensino de química, observamos a necessidade de novos referenciais teóricos e metodológicos que tornem esta atividade um campo de pesquisa cada vez mais vasto. Indo além dos referenciais de ensino e aprendizagem, propomos a utilização dos conceitos de cultura lúdica e cultura lúdica local na proposição e elaboração de novos jogos pedagógicos para o ensino de conceitos químicos. Dessa forma, corroboramos as ideias de Brougère1 , as quais o jogo é um local de construção e criação de uma cultura lúdica. Parece existir uma relação profunda entre o jogo e a cultura, o jogo e a produção de significados. Para o autor, para existir de

fato o jogo, é de fundamental importância a existência das relações sociais entre os participantes, de significados que possam ser socializados, de possibilidades diversas de interpretação, ou seja, a própria cultura. Existe, portanto, uma cultura lúdica que é um conjunto de procedimentos que tornam possível a realização do jogo, ou seja, ela corresponde a um conjunto de regras e significações próprias do jogo que o jogador adquire e domina no contexto de seu jogo. Essa cultura, assim como qualquer outra, não está pronta no individuo, pelo contrário, é o sujeito quem se apropria da cultura lúdica disponibilizada nas relações sociais e educativas. Neste sentido, entendemos que se faz necessário detectar a cultura lúdica local e a partir dela, elaborar e aplicar um jogo pedagógico para determinado conceito científico. Portanto, neste trabalho, por meio de questionários e entrevistas, detectamos a cultura lúdica local de discentes de escolas de diferentes regiões da cidade de Goiânia-GO, para, a partir dos resultados, elaborar e aplicar jogos correlatos. O pressuposto é que os jogos pedagógicos que se relacionem com a cultura lúdica local, terão mais êxito em termos de aprendizagem e facilidade de entendimento e relações sociais. Foram aplicados e analisados para este trabalho, cerca de 300 questionários de 4 escolas diferentes. Os resultados nos mostraram que é predominante o uso de jogos de cartas. Este tipo de jogo é citado em mais de 50% das respostas. Seguidas por jogos de tabuleiro e jogos eletrônicos, o que corrobora os resultados obtidos por Garcez e Soares2 , no estado da arte sobre jogos em ensino de química, isto é, os professores tendem a utilizar em maior quantidade, jogos de cartas para ensinar conceitos em química, por já entenderem, de maneira intuitiva que este é o tipo de jogo mais culturalmente imbricado nas relações sociais brasileiras. Tais tipos de jogos podem ser classificados como Agon e Alea, ou seja, jogos de competição que tem dependência também da sorte, essa classificação é baseada em um entendimento comportamental3 baseado na cultura expressa pela sociedade e manifestada em seus vários tipos de jogos e brincadeiras.

Produção de Podcast, Metodologia Ativa de Ensino Aprendizagem no estudo da Radioatividade

https://proceedings.science/p/120754

Luciana do Nascimento Rodrigues [1]; Thays Ferreira de Souza [2]; Ívina Langsdorff Santana [3]; Paulo Rogerio Garcez de Moura [3]

[1] Universidade Federal do Espírito Santo, Brazil; [2] PPGEnFis - Universidade Federal do Espírito Santo; [3] PPGQUI - Universidade Federal do Espírito Santo

Use of Digital Information and Communication Technologies (TDIC). Podcast as a method of active teaching from the elaboration and publishing of multimedia files in streaming platforms by the students.

Proposal of an investigative case to context Qualitative Analytical Chemistry subjects

https://proceedings.science/p/119431

Carolina Lourencetti [1]

[1] IFSP - Câmpus Matão

QUANTIFICAÇÃO DE NANOPARTÍCULAS DE PRATA EM UM PRODUTO FARMACÊUTICO POR ESPECTROFOTOMETRIA

https://proceedings.science/p/120581

Valéria Almeida Alves [1]; Luís Antônio da Silva [1]; Gabriel Souza Bernardes [1]; Richard Hermógenes Lima [1]

[1] Universidade Federal do Triângulo Mineiro

Spectrophotometry technique was used to quantify silver in an ophthalmic solution.
A standard solution of silver nanoparticles was synthesized. An analytical method was developed.

Quer que eu desenhe? Fazendo arte com a química

https://proceedings.science/p/119863

Rosana Petinatti da Cruz [1]

[1] UFRRJ

QUÍMICA ANALÍTICA PARA O ENSINO MÉDIO: UM NOVO TEMPO UMA NOVA ABORDAGEM

https://proceedings.science/p/119683

Ana Paula dos Santos Xavier Ferreira [1]; Ariele Oliveira Franco [2]; Amauri Souza [3]; Carla Patrícia de Oliveira Ferreira Melo [4]; Eric Marsalha Garcia [5]; Hosane Aparecida Taroco [6]; Mayara Neves Santos Guedes [7]; Miriã Cristina Pereira Fagundes [8]; Luisa Del Carmen Barrett Reina [9]; Yesenia Mendoza García [10]; Altamir Fernandes de Oliveira [11]; Julio Onésio Ferreira Melo [2]

[1] Universidade federal de são João del Rei campus sete lagoas; [2] Universidade Federal de São João Del Rei; [3] Universidade Federal de São João Del Rei - Campus Sete Lagoasdo Oeste do Pará; [4] Universidade Federal de São João del-Rei - Campus Sete Lagoas; [5] Universidade Federal de São João dei rei; [6] Universidade Federal de São João del Rei; [7] Universidade Federal do Oeste do Pará; [8] Universidade Estadual de Santa Cruz; [9] Universidade Federal de Mato Grosso; [10] Universidade Federal de Alagoas ; [11] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Analytical Chemistry for high school, a new time a new approach. The study of chemistry is very important in the formation of good professionals, because it permeates in almost all areas of knowledge.so the importance to arouse in students the curiosity to learn chemistry

Química com Agrotóxicos: Desenvolvendo uma oficina para ensinar o conteúdo Haletos Orgânicos

https://proceedings.science/p/120618

Carlos Fernando de Souza Santos [1]; Isabela Torres Oliveira [1]; Cleyton Bispo Paulino [1]; Stefany Dias Oliveira Soares [1]; Roberta Menezes Santos [1]

[1] Universidade Federal de Sergipe

Report of experiences lived in a thematic workshop; Present the relevance of the theme Pesticide as a proposal for the teaching of content Organic Halides; Environmental awareness.

Química com poesia: análise da leitura e influências de experimentos na apropriação de conceitos

https://proceedings.science/p/120013

Milene da Silva [1]; Wilmo Ernesto Francisco Junior [1]

[1] Universidade Federal de Alagoas

We provide a teaching strategy that combined a poem about chemistry and experiments in order to discuss concepts presented in the text.

Relato de Experiências: Oficina de síntese de óxidos de ferro na presença de resíduo de manga para estudantes da educação básica

https://proceedings.science/p/120186

Marluce Oliveira da Guarda Souza [1]; Lucas Malone Ferreira de Castro [2]

[1] UNIVERSIDADE DO ESTADO DA BAHIA; [2] UNIVERSIDADE FEDERAL DA BAHIA

A preocupação com a formação do cidadão é crescente demandando ações no sentido contribuir para melhorar a educação da população. Faz-se necessário, nesse contexto, aproximar a universidade das distintas comunidades considerando a tríade ensino, pesquisa e extensão e correlacionando os saberes acadêmicos e populares, sendo, por exemplo, da Educação Básica. Assim, o presente trabalho faz um relato sobre uma oficina de síntese de óxidos de ferro pelo método da combustão utilizando o resíduo de manga como reagente auxiliar, ministrada para estudantes do 9º ano de duas escolas de Ensino Fundamental II de Salvador. Tal oficina abordou, em conjunto com o experimento, a discussão sobre os conteúdos de reações químicas, termoquímica e química ambiental, destacando aproveitamento de resíduos. Inicialmente houve uma apresentação das instalações de um Laboratório de Pesquisa em Química Aplicada, abordando aspectos de segurança, apresentando equipamentos e reagentes utilizados, destacando informações dos rótulos e correlacionando com os conteúdos correspondentes. Em seguida, foi realizado um experimento com a reação de síntese de óxidos de ferro por combustão (Figura 1), com e sem a adição do resíduo de manga, enfatizando as diferenças observadas no momento da síntese e os aspectos físicos do produto obtido. Os estudantes demonstraram entusiasmo com o ambiente laboratorial, bem como com o experimento. As intervenções feitas ao longo da oficina se mostraram efetivas na consolidação dos conteúdos abordados, visto que os estudantes responderam de forma efetiva

aos questionamentos propostos. A oficina mostrou-se como uma alternativa válida para auxiliar no ensino de química na Educação Básica e para aproximação entre universidade-escola-comunidade.

Ressignificação dos conceitos de química no ensino médio, através do assunto eletronegatividade

https://proceedings.science/p/120447

Marco Antônio Moreira de Oliveira [1]; Marcelo Vieira Migliorini [2]

[1] Universidade Estadual do Rio Grande do Sul - UERGS; [2] Engenharia de Bioprocessos e Biotecnologia / Unidade Santa Cruz do Sul / Universidade Estadual do Rio Grande do Sul e PROPPG / MESTRADO EM DOCÊNCIA EM STEM / Guaíba / Universidade Estadual do Rio Grande do Sul

Conceptual resignification, providing meaningful learning, with real experimentation, so that electronegativity is the conceptual basis for understanding Chemistry, using Educational Product created.

Studies of the application of Virtual Learning Object in focus: analysis of formaldehyde present in hair straighteners

https://proceedings.science/p/119715

Gustavo Augusto Assis Faustino [1]; Victor Borges Marinho Silva [1]; Brunno André Ruela [1]; Amanda Alves Arrais de Morais [1]; Thais de Souza Lima [1]; Anna Maria Canavarro Benite [2]; Claudio Roberto Machado Benite [1]

[1] Universidade Federal de Goiás; [2] Universidade Federal de Goiás

The study shows how Virtual Learning Object can help in Chemistry teaching and in the critical formation of students regarding the indiscriminate use of hair straighteners.

Sustentabilidade e protagonismo na aprendizagem mediada pela educação ambiental em experimentos de química geral

https://proceedings.science/p/120233

Jussara Lopes de Miranda [1]; Hiasmin Christine Kurrle Pinheiro Sodre [2]; Thais Delazare [3]; Paula Santos [3]

[1] INSTITUTO DE QUÍMICA - UFRJ; [2] INSTITUTO DE QUIMICA- UFRJ; [3] INSTITUTO DE QUÍMICA-UFRJ

Buscando inserir a ideia de associação da sustentabilidade com o protagonismo dos próprios alunos de graduação de Química e de Engenharia, foi elaborado um projeto compartilhado para a gestão ambiental das aulas experimentais de Química, assim como o tratamento de efluentes químicos gerados. Foi proposta também a substituição dos experimentos existentes por outros de menor grau de toxicidade visando promover a educação ambiental1 mediante a discussão dos temas associados, assim como contribuir para o processo formativo de profissionais mais conscientes das suas responsabilidades socioambientais. O tratamento de efluentes de rejeitos químicos de aulas experimentais de Química Geral foi realizado pelos próprios alunos da disciplina, com a prévia contextualização ambiental, mediada pelos docentes, com discussão da importância e conteúdo da Resolução do CONAMA 430/2011, que dispõe sobre as condições e padrões de lançamento de efluentes2. O tratamento do rejeito dessa aula, além de trazer economia, contribuiu para que os alunos elaborassem uma nova perspectiva de responsabilidade ambiental. Ademais, os alunos puderam experienciar uma situação em que tiveram que resolver um problema, trabalhando em equipe para buscar uma solução. A análise e substituição de experimentos existentes por outros de menor grau de toxicidade está em fase de desenvolvimento e tem como objetivo principal a substituição de reagentes e reações envolvidas nas aulas de Química Geral por outros menos tóxicos, sem que haja perda qualitativa de aprendizado. Para atingir este objetivo, acompanharam-se as aulas laboratoriais da disciplina Química Geral experimental durante um semestre a fim de analisar e selecionar os procedimentos de maior grau de toxicidade que poderiam ser substituídos. Os critérios para esta seleção foram os seguintes: a) grau de exposição a reagentes de alto grau de toxicidade, b) manutenção dos objetivos didáticos do aprendizado, c) disponibilização de reagentes e procedimentos nos laboratórios da Universidade. Dessa forma, foram selecionados dois experimentos, onde se utilizam compostos de 1) arsênio e 2) cianeto.

Teaching-as-research: Proposal of an active methodology for the teaching of Biochemistry

https://proceedings.science/p/120244

Elisabete de Avila da Silva [1]; Udo Eckard Sinks [1]; Romuel Barros Costa e Silva [1]; Daiana Kaminski de Oliveira [2]
[1] UNIPAMPA; [2] FURG

According to QUADROS and MORTIMER (2014) when science teachers organize their class around concepts, not relating them to the social context, nor valuing the role of students in the construction of their knowledge, end up promoting a mechanical and contentious learning dislocated from reality and thus inhibiting critical thinking. To combat this form of learning, since the 1970s, methodologies are proposed using the student's social context, activity, which combine theory and practice turning the student a more active part of the learning process. Inquiry-based learning is an approach which emphasizes the student's role in the learning process. Rather than the teacher telling students what they need to know, students are encouraged to explore the material, ask questions, and share ideas. Inquiry-based learning is known in literature, ZÔMPERO e LABURÚ (2018), also as teaching by discovery, learning by projects, teaching by question, problem centered teaching. Inquiry-based learning and teaching-as-research enables the improvement of students' reasoning and cognitive abilities, the improvement of working (learning) in a team, besides enabling them to understand the nature of scientific work. Realizing the need of an alternative teaching metodology that attends demands of science teaching, this works develops a proposal to realize teaching-as-research in the biochemistry class in the graduate course of chemistry at Universidade Federal do Pampa (UNIPAMPA) during the first semester in 2020. The proposed activity will be divided into three distinct parts: First, students will receive a research problem which should be done throughout the semester. During the semester students should find answers using books, articles and other means, in addition to information presented in biochemistry classes. Second, students will propose answers and should socialize/discuss their ideas with other students in dates defined in the class schedule. Third, students should write abstracts with the findings/proposals and present them at the 1st Investigative Exhibition of Biochemistry of UNIPAMPA, to be held at the end of the semester. Results will be observed and analized during the realisation of our teaching proposal by questionnaires before and after writing the aforementioned abstracts. We expect to show that our students are able to construct knowledge, develop their capability in biochemistry and appropriate more specific chemistry skills. By this activity, we expect that students develop autonomy to build a new look at phenomena that are presented in the biochemistry class, linking scientific concepts to effects in vivo. In addition, as the graduate course of chemistry trains teacher to act in primary and secondary education, it is also intended that teaching-as-research will be part of the day-to-day toolbox of those future teachers, who, once graduated, can use this approach of teaching in their classes.

The Environment and Color Chemistry

https://proceedings.science/p/119600

Mariana Oliveira Fraga [1]; Jheyze Tauane Nunes de Aquino [1]; Yasmim Morais Silva [1]; Marlene Viana dos Santos [1]
[1] Universidade Federal de Sergipe

This paper was based on the didactic proposal of the Three Pedagogical Moments (3MPs), with the aim of inserting a new teaching concept on the textile dyeing chemistry and the environmental issue.

The Importance of Interdisciplinarity in the Teaching of Environmental Chemistry: A Look Through Chemistry Students at the State University of Para

https://proceedings.science/p/119546

Ramon Gabriel Pinho Botelho dos Santos [1]
[1] Universidade do Estado do Pará

1. The importance of interdisciplinarity in the teaching of environmental chemistry; 2. Chemistry students' point of view from the State University of Pará.

Ticx0092s em química: Desenvolvimento de programas e suas aplicações

https://proceedings.science/p/120047

Elisangela Costa Santos [1]; Ermesson Lima dos Santos [2]; Dalton Serafim de Oliveira [3]
[1] Instituto Federal de Educação, Ciências e Tecnologia de Alagoas - Campus Penedo; [2] Instituto Federal de Educação, Ciências e Tecnologia de Alagoas; [3] Universidade Federal de Alagoas

Labreal is an augmented reality game.
VRLabe is a virtual reality game.
QuizQuimica is a trivia-style game (questions and answers).
All three programs were registered as computer programs at the INPI.

Uma oficina virtual com alunos da Educação de Jovens e Adultos: A correta utilização da água sanitária no combate ao COVID-19

https://proceedings.science/p/120497

Gizelle Inácio Almerindo [1]; Felipe M. Müller [1]; Julia Spohr Grigolo [1]; Beatriz Batista Warmling [1]; Sophia Miskowiec Ferreira da Silva [1]; Nicoli Fernanda Veyra [1]; Jaíne Santos de Moura [1]; Anelise Ehrhardt [1]; Patrícia F. S. Costodio [1]
[1] Universidade do Vale do Itajaí

- Significant potential for virtual workshops during the pandemic;
- The dilution of bleach is not yet known to everyone;
- The Word Cloud highlighted scientific terms addressed.

Uma Proposta de Robótica Educacional Aplicada ao Ensino de Titulações Ácido-Base

https://proceedings.science/p/120409

Iterlandes Machado Junior [1]; Efraim Lázaro Reis [2]; César Reis [2]; Odilaine Inácio de Carvalho Damasceno [3]; Per Christian Braathen [4]
[1] UFV (Universidade Federal de Viçosa) - Campus Universitário; [2] UFV (Universidade Federal de Viçosa) - Campus Viçosa; [3] Colégio de Apliação (CAp-COLUNI) / UFV (Universidade Federal de Viçosa) - Campus Viçosa; [4] UNIVIÇOSA

This study had as focusthe construction of an automatic titrator of low cost and easy acquisition. For that, the Open Sourse Arduino platform was used in order to enable the development of research activities in the teaching of chemistry. The acquisition of the experimental data was performed via Bluetooth through integration with the Smartphone and via USB cable directly to the Microsoft Excel worksheet. The results were compared with the classical potentiometric titration, showing no statistically significant differences with the test applied at 95% confidence level. The purpose of the research teaching proposal was to experimentally determine the pKa value of captopril, that it is used with antihypertensive drug.

This active learning methodology privileges work in collaborative groups and student participation in the construction of their knowledge. Further research on the possibilities of teacher training through the application of this instrument and other chemistry projects with Arduino in professional qualification courses at undergraduate and/or postgraduate level needs tobe problematized. The complete description of this project is available in a dissertation published on the official page of PROFQUIUFV

Highlights

- A proposal to use educational robotics to teach was implemented
- Through connections between pH module, peristaltic valve and Arduino® platform, a potentiometric titration is operated automatically

Why the Chaos? A Reflection on the Concept of Entropy

https://proceedings.science/p/120341

Ítalo Macêdo Gonçalves [1]; Roberta P. Dias [2]; Ana Paula Souza [2]
[1] Universidade Federal de Pernambuco - Campus Agreste; [2] Universidade Federal de Pernambuco - UFPE

The concept of entropy is approached superficially in undergraduate chemistry courses. Often, the teachers in formation elaborate a conceptual model about entropy that can be mistaken.

QuíNutri: uma proposta de divulgação científica para a química de alimentos.

https://proceedings.science/p/119460

Guilherme Sippel Machado [1]; Dayane Carla Brinhosa [1]
[1] Universidade Federal do Paraná / Campus Pontal do Paraná - Centro de Estudos do Mar

Uma dieta balanceada deve combinar variedade e quantidades apropriadas de alimentos à idade e ao grau de atividade física de cada indivíduo. Visando contribuir para a divulgação de informações úteis e cientificamente comprovadas sobre a química de alimentos, baseando-se na bioquímica de alimentos, este trabalho buscou abordar a importância da nutrição e do conhecimento sobre a identificação das propriedades dos alimentos, criando um canal de divulgação científica utilizando um perfil em uma rede social de compartilhamento de fotos e vídeos (Rede social: Instagram®; nome do perfil: @tccquinutri - uma sigla misturando química, nutrição e o trabalho de conclusão de curso vinculado), conjuntamente com uma pesquisa realizada com alunos do Ensino Médio (EM) em uma instituição parceira da rede estadual de ensino de Pontal do Paraná.

A coleta de dados com os alunos foi realizada com o intuito de entender mais sobre como eles se alimentam e quais informações prévias tinham sobre o assunto abordado, observou-se que muitos alunos possuíam hábitos alimentarem ruins para a saúde, como por exemplo, com alto consumo de refrigerantes, doces e frituras no dia-a-dia. Depois de coletados os dados, um cronograma para postagens semanais na rede social foi elaborado, dentre alguns assuntos selecionados estavam as classes de alimentos dos carboidratos, lipídeos (gorduras saturadas, insaturas e trans) e aminoácidos e proteínas, exemplos das postagenspodem ser vistos na figura ao lado. Os textos das postagens eram selecionados e produzidos fundamentados na base teórica sobre a química dos alimentos, sendo as imagens produzidas pelos autores ou buscadas em sites de compartilhamento livre.

O conhecimento adquirido após a estratégia de divulgação na rede social pelos alunos que seguiram o perfil foi avaliado por meio de entrevistas com estes estudantes, sendo que um retorno bastante positivo sobre a estratégia e um melhor entendimento sobre a correta alimentação foi observado com a maioria dos alunos, inclusive com mudanças nos hábitos alimentares, como pode ser observada nas citações a seguir de alunos do primeiro ano e terceiro ano do EM, respectivamente: “Tive conhecimento de assuntos que desconhecia, como por exemplo, a existência de gorduras boas em alguns alimentos” e “Tive conhecimento sobre refrigerante, a quantidade de açúcar que ingeria e me conscientizei, passando a ingerir menos”. Ao todo foram 68 seguidores do perfil na rede social, desses seguidores, 10 foram alunos do colégio.

Highlights

- QuíNutri: a scientific dissemination proposal for food chemistry.
- Social network profile for scientific dissemination.
- Observation of students eating habits.
- Nutritional information based on food biochemistry.

Físico-Química - FIS

Influência da nanocelulose na liberação de hidroxicloroquina mobilizada em filmes de pectina

https://proceedings.science/p/120431

Giovana C Zambuzi [1]; Júlia da Silva Forster [2]; Camilla Camargos [3]; Maira Peres Ferreira-Duarte [4]; Osvaldo de Freitas [4]; Camila Rezende [3]; Kelly Francisco [2]

[1] Universidade Federal de São Carlos; [2] Departamento de Ciências da Natureza, Matemática e Educação / Universidade Federal de São Carlos; [3] Universidade Estadual de Campinas; [4] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP)

HCQ-pectin films with and without nanocellulose were obtained; HCQ-pectin films containing nanocrystals showed a more homogeneous surface; Nanocrystals decreased the HCQ release in the aqueous phase.

Adsorption and stability study of self-assembled monolayers on calcite (CaCO3)

https://proceedings.science/p/120533

Caroline Aoki [1]; Paulo Miranda [2]

[1] Universidade de São Paulo; [2] IFSC-USP (Universidade de São Paulo)

Fabrication of stearic acid monolayers on calcite surface

Carbonization effect of sugarcane bagasse in the atrazine and methylene blue adsorption

https://proceedings.science/p/119456

Gabriel Cabral da Fonseca [1]; Marilene Silva Oliveira [1]; João Carlos Perbone de Souza [1]

[1] Instituto Federal de Educação, Ciência e Tecnologia Goiano

An extensive sugarcane planting is necessary due to the high demand for alcohol production, which after processing to obtain the dense broth, millions of tons of bagasse are generated. Many papers have been done to show that porous materials, such as activated carbon, produced from agroindustrial residues, have high adsorptive capacity in aqueous solutions. The aim here was to produce activated carbon from sugarcane bagasse to evaluate its adsorptive capacity in atrazine (ATZ) and methylene blue (MB) solutions. Sugarcane bagasse was collected at the Cambui Industry in Goias state, was dried at 100 ºC and submit to carbonization (thermal activation), for 3 and 5 hours at 200 ºC (CA3 and CA5, respectively). Samples CA3 and CA5 were characterized: (1) Fourier Transform Infrared Spectroscopy (FTIR) to analyze the changes in the functional groups of the compounds present in the material during carbonization; (2) Scanning Electron Microscopy (SEM) where the micrographs showed that the quantity of particles decrease and the porous increase with carbonization time and (3) thermogravimetry (TG), which shows a mass loss at 350 ºC related to 80 % cellulose/hemicellulose composition. To the ATZ adsorption analyses, 10 mL (5 – 50 mg L -1) was added to 10 mg of CA3 and CA5 sample and stirred at 150 rpm for 24 hours. For MB, 50 mL (5 – 40 mg L -1) was added to 50 mg of CA3 and CA5 sample and stirred at 150 rpm for 24 hours. The solutions were filtered through a 0.45 µm pore size syringe filter and analyzed by UV-Vis spectrophotometer (λATZ = 222 nm; λMB = 664 nm). For residual concentration calcule was done by standard curve equation (R2 ATZ = 0,999; R2 MB = 0,999). The isotherms (Figure 1) and qe values (Table 1) show that CA3 has the best performance on adsorption to the MB (qe = 33,08 mg g - 1). The carbonization effect was observed on the ATZ adsorption, when the qe value increase from 22,62 to 31,87 mg g -1 , which are associated to increase of carbonization time, creating a number of available sites for molecular adsorption1 , and decreasing on particle size raising the specific surface area2 . The Langmuir isotherm can adequately represent the data obtained, which demonstrate the high correlation coefficients3 .

Descoloração do azul de metileno (AM) por plasma frio: efeitos de sulfato de sódio e pirrotita (FeS) como catalisador.

https://proceedings.science/p/120525

Maria Luiza Rodrigues Soares [1]

[1] Universidade Federal de Santa Catarina

MB was degraded using non-thermal plasma and pyrrothyte as a catalyst, sodium sulfate was used as an as a model ionic specie to mimic wastewater ionic charge to study the effect of ions in solution.

Efeitos do pH na síntese hidrotérmica do fotocatalisador BiVO4 e avaliação de suas propriedades fotocatalíticas

https://proceedings.science/p/120627

Caroline Santana dos Santos [1]; Beatriz Caetano Benuto [1]; Rafael Junqueira Leal [1]; Raul Zanchet [1]; Marcelo Zampieri [1]; Roberta Antigo Medeiros [1]; Roberto de Matos [1]

[1] Universidade Estadual de Londrina

BiVO4 was synthesized by hydrothermal method. The increase in the pH of the precursor solution of BiVO4 favors the monoclinic phase, which showed greater photocatalytic efficiency under visible light.

Electrocatalytic activity toward hydrogen peroxide of a hybrid film contaning silicotungstic acid

https://proceedings.science/p/120644

Victória de Oliveira Margarido [1]; Julia Helena de Paula [1]; Adriano Lopes de Souza [1]; Kelly Francisco [1]

[1] Universidade Federal de São Carlos

A hybrid film containing silicotungstic acid (HSiW) and 3-aminopropyltriethoxysilane was prepared. This film showed electrocatalytic activity toward hydrogen peroxide at -0.14 V vs. Ag/AgCl.

Electrochemical Stability Assessment of CdTe Quantum Dots Immobilized on Gold Surfaces

https://proceedings.science/p/120375

Adriana Soares de Carvalho [1]; Adriana Fontes [2]; Rogério Tavares Ribeiro [3]

[1] Universidade Federal de Pernambuco/Departamento de Química Fundamental; [2] Universidade Federal de Pernambuco - UFPE; [3] MInT Consultoria em Materiais e Inovação Tecnológica LTDA

Application of cyclic voltammetry to study the stability of quantum dots. Influence of functional groups on the electrochemical stability of quantum dots.

Estudo teórico da degradação de compostos orgânicos voláteis em superfícies de TiO2

https://proceedings.science/p/120056

João Batista Lopes Martins [1]; Gustavo Olinto da Silva [1]

[1] UnB

Hidrocarbonetos aromáticos conhecidos por BTEX (benzeno, tolueno, etilbenzeno e isômeros de xileno) encontrados em reservas de petróleo e gás natural, cosméticos e solventes são contaminantes severos1,2. Desta forma, propiciar a fotocatálise desses poluentes seria uma boa forma de mitigar o impacto ambiental existente. É então fundamental alcançar catalisadores eficientes, estáveis e de baixo custo. Dentre os quais, a superfície (101) do dióxido de titânio (TiO2), na forma anatase, se apresenta como opção conveniente3. Entretanto, a anatase possui suas limitações, como a perda da energia absorvida como recombinação do par e-/h+4, e a ausência de atividade na presença de luz solar. Uma maneira de evitar tais imperfeições é a dopagem substitucional do catalisador. Assim, alterando suas características da forma desejada, seja por dopagem catiônica, aniônica, ou co-dopagem. Desta forma, este trabalho busca investigar a viabilidade de inserção de átomos de vanádio e nitrogênio como dopantes substitucionais, através da relação entre parâmetro de Hubbard (GGA+U) e band gap. Também é importante determinar o tipo de dopagem mais eficiente na adsorção de moléculas de tolueno e etilbenzeno. Na calibração do parâmetro de Hubbard, ao variar o termo de interação elétron-elétron (U), altera-se o valor de intervalo entre banda de valência e banda de condução (gap). Correspondente ao intuito de corrigir para os valores experimentais da literatura. Foram calculadas as energias de adsorção de etilbenzeno e tolueno nas superfícies de TiO2 (101) “puro”, dopado com nitrogênio, dopado com vanádio, e co-dopado com nitrogênio e vanádio, pelo funcional PBE, num sistema de condições periódicas de ondas planas. Os cálculos de adsorção mostraram que o tolueno adsorve com maior energia de interação na superfície de dióxido de titânio dopada com vanádio, enquanto para o etilbenzeno a superfície dopada com nitrogênio seria a mais indicada. 1. Masih A, Lall AS, Taneja A, Singhvi R. India. Chemosphere 2017; 176:8–17. 2. Bielen A, Šimatović A, Kosić-Vukšić J, et al. Water Research 2017; 126:79–87. 3. Lazzeri M, Vittadini A, Selloni A. Physical Review B 2001; 63. 4. Hashimoto K, Irie H, Fujishima A, Japanese Journal of Applied Physics 2005; 44:8269–85.

Estudo termodinâmico e cinético para biocarvão de Avena a partir de biomassa residual

https://proceedings.science/p/120425

Janaina Pontes da Silva [1]; Cristian Pessotto [1]; Bárbhara Talyssa Michels [1]; Fernanda Maria Xczepaniak [1]; Jaqueline Nicolini [1]; KELLER NICOLINI [1]

[1] Instituto Federal de Educação, Ciência e Tecnologia do Paraná - IFPR

The initial rate of TY adsorption in AB is inversely proportional of the batch assays temperature.
BC produced show exothermic and non-spontaneous adsorption, involving valency forces.

Experimental factors that influence in the yield and reproducibility of gold nanorods synthesis and SERS spectroscopy performance

https://proceedings.science/p/119984

Flávia Campos Marques [1]; Débora Guimarães Oliveira [1]; Gustavo Fernandes Souza Andrade

[1] UFJF

Gold nanorods synthesis yield is strongly influenced by surfactant origin and temperature control. Removing surfactant excess by centrifugation/re-suspension is essential for SERS performance. Optimal conditions for the SERS spectra of the cyanine dye IR-820 are reported.

Extração de óleo essencial de Syzygium aromaticum através de hidrodestilação

https://proceedings.science/p/120761

Daniel Alves Cerqueira [1]; Cassia Cardoso [1]; Janaína Placedes [1]

[1] Universidade Federal do Triângulo Mineiro

Extraction of Syzygium aromaticum essential oil by hydrodistillation. Distillation for obtaining antifungal essential oil. Mass yield of 5.5% for the oil. Recovery of 95% of the total oil in 120 min.

Interaction of self-assembled chitosan nanoparticles and phospholipid membranes at air-water interface

https://proceedings.science/p/120500

Rafael de Oliveira Pedro [1]; Paulo Miranda [2]

[1] Universidade do Estado de Minas Gerais; [2] IFSC-USP (Universidade de São Paulo)

The binding of chitosan derivatives to phospholipid monolayers depends on the type of lipid headgroup

Magnetic Composite MnFe2O4 / Biochar for Removal of Rifampicin Antibiotic from Aqueous Solution

https://proceedings.science/p/119525

Denise M. V. Cursino [1]; Pollyanna V. S. Lins [1]; Lucas Melli [1]; Carmem Lucia de Paiva Silva Zanta [1]; José L. S. Duarte [1]

[1] Universidade Federal de Alagoas

In this work a magnetic composite was synthesized. This composite is formed by sugarcane biomass, which has undergone a hydrothermal treatment, and is supported with iron and manganese metal ions. This composite was used in the activation of sulfate radicals presentfromsodium persulfate solution, since sulfate radicals are known to have a higher oxidation potential than persulfate. In addition to the kinetics of sulfate, which is faster than the kinetics of persulfate. This activation has the contributionof the UV lamp, helping with the activation of the radicals. The synthesized composite was characterized by Fourier Transform Infrared (FT-IR) and Xray Diffraction (XRD)(Fig. 1A and B), then was tested in the treatment of emergingpollutantrifampicin effluent, an antibiotic used mainly in the treatment of tuberculosis and can be excreted from the human body in various forms and still in its active form. This

study is due to the fact that conventional Effluent Treatment Stations (WWTP) do not have technology in their facilities to eliminate this drug in its entirety.Onlya partof this drug is removed, where most of it goes into the waterways, causing imbalances in the ecosystems to pass through, and may even cause resistance to the bacterium responsible for tuberculosis, Mycobacterium tuberculosis or Bacillus de Koch (BK). The system containing the MnFe2O4 / Biochar (0.04g) persulfate (4mM) and UV light composite achieved approximately 94% removal(Fig. 1C)of the rifampicin antibiotic

Microwave Hydrothermal Synthesis, Characterization, and Dye Photocatalytic Performance of TiO2 nanoparticles.

https://proceedings.science/p/120522

Rafael Guerra Ferreira [1]; Tamara Pereira da Silva [1]; Douglas Santos Monteiro [2]
[1] Instituto de Ciência, Engenharia e Tecnologia / Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Universidade Federal dos Vales do Jequitinhonha e Mucuri

- Nano-TiO2 (cuboids, rods, triangles) were successfully prepared using microwave heating.
- Microwaves reduced synthesis time by 60%.
- Nanoparticles exhibited excellent dye photodegradation.

Multipath Variational Transition State Theory for Reactions with Flexible Molecules

https://proceedings.science/p/119800

Tiago Vinicius Alves

Nitreto de Carbono Grafítico Sintetizado a partir da Decomposição Térmica da Uréia e seu uso como Fotocatalisador.

https://proceedings.science/p/120531

Everton Wilker [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

g-C3N4 was successfully synthesized and 2D sheets were obtained.
The nanomaterial removed of about 76% of the dye.

Observation of mixed mode oscillations in the chlorate-nitrous acid-iodine/iodide oscillating reaction

https://proceedings.science/p/119607

Emily Vidal Monteiro [1]; Roberto de Barros Faria [1]
[1] Universidade Federal do Rio de Janeiro

Mixed mode oscillations were observed for the first time in the recently discovered chlorate—nitrous acid—iodine/iodide oscillating reaction.

On the mechanism of aqueous nitrogen species produced by non-thermal air plasma

https://proceedings.science/p/120366

Pericles Inacio Khalaf [1]
[1] UTFPR

Partitioning of Ametryn in aqueous two-phase systems

https://proceedings.science/p/120416

João Otávio Ferreira [1]; Davi Siqueira da Silva de Souza [2]; Julia Helena de Paula [1]; Adriano Lopes de Souza [3]; Kelly Francisco [3]

[1] Universidade Federal de São Carlos/ Centro de Ciências e Tecnologias para Sustentabilidade - DFQM-So; [2] Universidade Federal de São Carlos/ Centro de Ciências Agrárias - DCNME-Ar; [3] Universidade Federal de São Carlos/ Centro de Ciências Agrárias - DCNME-Ar/ Centro de Ciências e Tecnologias para Sustentabilidade - DFQM-So

Use of aqueous two-phase systems (ATPS) to separate Ametryn from contaminated water sources. Quantification of Ametryn in aqueous medium by HPLC technique after partitioning in ATPS.

Physico-chemical and nutritional evaluation of Pachira Aquatica Aublet nuts and production of biodiesel from oil

https://proceedings.science/p/120103

Keurison Figueredo Magalhães

Polydialyldimethylammonium chloride (PDADMAC) and cationic chitosan as carbonate rock wettability inverters for enhanced oil recovery (EOR)

https://proceedings.science/p/120220

Agatha Densy dos Santos Francisco [1]; Daniel Grassechi [1]; Regina Nascimento [1]

[1] Universidade Federal do Rio de Janeiro

Cationic polymers on EOR may act to improve the sweeping efficiency, reduce interfacial tension and mainly as wettability inverters, increasing the oil recovery factor.

Problem-based learning: the use of prototypes operating in real thermodynamic cycles for teaching thermodynamics.

https://proceedings.science/p/120088

Ronaldo Duarte Leal [1]; Yuji Watanabe [1]; Rodrigo de Paula [1]

[1] Universidade Federal do Recôncavo da Bahia

Carnot and Stirling Thermodynamic cycles for teaching Physical-Chemistry. Stirling cycle as an example of a real thermodynamic cycle allowing students to calculate all state functions in each step.

Remoção do corante alizarina de soluções aquosas utilizando porongo como biossorvente

https://proceedings.science/p/120424

Kethleenn Drusina de Lima [1]; Karin Cristina Leonardi [1]; KELLER NICOLINI [1]; Jaqueline Nicolini [1]

[1] Instituto Federal de Educação, Ciência e Tecnologia do Paraná - IFPR

Biosorption (2 < n < 10) indicate low heterogeneity. Linear biosorption (RL = 1) favorable to the monolayer model. The kinetic model indicates that sorption occurs at the solid / liquid interface.

SERS Effect Investigation of CdTe Quantum Dots: a Comparative Study with Ag and Au Nanoparticles

https://proceedings.science/p/119533

Kelly Aparecida Silva Souza [1]; Luciano Sindra Virtuoso [1]; Ana Paula Pereira Alves [1]
[1] Universidade Federal de Alfenas - MG

The Surface Enhanced Raman Scattering (SERS) effect has been applied as a powerful analytical technique highly sensible for trace concentrations detection of biological analytes. Specifically, the SERS effect is more pronounced when the analyte is adsorbed on Ag and Au metallic nanoparticles (NPs) substrates [1]. Nevertheless, semiconductors nanomaterials have been explored as an alternative substrate for SERS effect [2]. CdTe QDs are already applied as biological markers and its use as SERS substrate brings an innovative and simple analytical tool for analyzing complex matrices. In this work, we have studied the comparative SERS effect of CdTe QDs with Ag and Au NPs deposited on glass plates previously functionalized with (3-aminopropyl)triethoxysilane (APTES), and using crystal violet (CV) 1x10-3 mol L -1 as the analyte absorbed on the respective nanomaterial substrate. **Palavras Chave:** SERS, Quantum Dots (QDs), Gold nanoparticle, Silver nanoparticle, CdTe QDs

Structural Characterization of Dental Glasses by Multinuclear Solid State NMR

https://proceedings.science/p/119413

Guilherme Augusto Ferreira [1]; Viviane Oliveira Soares [2]; Lais Dantas Silva [3]; Edgar D. Zanotto [3]; Hellmut Eckert [1]
[1] Universidade de São Paulo; [2] Universidade Estadual de Maringá; [3] Universidade Federal de São Carlos

Solid State NMR of multicomponent silicate glasses functionalized by the incorporation of metal oxides revealed different spatial distributions of the network former and modifier species.

Study of the Kinects of Photodegradation of Opuntia Dillenii in different acids

https://proceedings.science/p/120093

Robson Filho [1]; Ricardo Lima Guimarães [1]; Arthur Neves [1]; Nayally Rayany Soares Marques [1]; Edson Ednaldo da Silva [1]
[1] Universidade Federal de Pernambuco - UFPE

The objective of this work was obtaining extracts in aqueous and ethanolic medium from the fruit of the erect prickly pear (Opuntia dillenii) in different acids and study their photodegradation kinetics in UVC radiation and analysis by UV-Vis spectroscopy. In water, the best result of resistance to degradation was observed in the absence of acid, meanwile, in ethanol, the best results were observed with the use of ascorbic acid as a co-pigment and with hydrochloric acid.

Unveiling PA11 degradation utilized on flexible risers using XPS spectroscopy.

https://proceedings.science/p/120460

Frederico Gonçalves de Albuquerque Dias [1]; Maria Luiza Miranda Rocco [1]; Amanda Garcez da Veiga [1]; Marysilvia Ferreira da Costa [1]; Antonio Pedro Gomes [1]
[1] Universidade Federal do Rio de Janeiro

Pure and used PA11 were analyzed using XPS and FTIR. It was found that most of the reactions were promoted by water in contact with the polymer. Other fluids don't seem to alter PA11 composition.

Fotoquímica - FOT

Effect of metal complexation on the PDT application of curcumin derivatives against Sporothrix brasiliensis yeasts

https://proceedings.science/p/119666

Bruna Martins de França [1]; Lucieri Olegario Pereira Souza [1]; André Luis Souza dos Santos [1]; Josué Sebastián Bello Forero [1]; Rodrigo José Corrêa [1]

[1] Universidade Federal do Rio de Janeiro

Energy recovery from wastewater produced by cassava processing using Ni(x%)-TiO2 as photocatalysts

https://proceedings.science/p/119845

Klebson Souza Santos [1]; Luciana Almeida da Silva [2]; Paula Aparecida Lima Lopes [2]

[1] Universidade Estadual de Feira de Santana; [2] Universidade Federal da Bahia

>It was possible to produce clean fuels (H2 and C2H4) from wastewater. >An AOP performed in oxygenfree atmosphere is a promising way to remediate pollutants, converting into friendly fuels.

IR-820 SERS AND SEF PERFORMANCES IN ALGINATE SILVER NANOPARTICLES AND IN CALCIUM-Ag-ALGINATE POROUS

https://proceedings.science/p/119669

Mari Ferreira Nicolas [1]; Marcia Laudelina A. Temperini [1]; Giordano Paganoto [1]; Jayr Marin [1]

[1] Universidade de São Paulo

Template synthesis was made by Ag@ALG embedded in calcium alginate. The dye IR-820 was used for obtaining both the enhanced Raman (SERS) and enhanced fluorescence (SEF) at 633 and 785 nm.

Light induced CO release of a new water soluble manganese(I) compound

https://proceedings.science/p/119825

Vinícius Acir Glitz [1]; Bruna Luiza Auras [2]; André Amorim [2]; Herculys Bernardo Jorge [1]; Ademir Neves [1]; Rosely Aparecida Peralta [1]

[1] Universidade Federal de Santa Catarina; [2] Departamento de Química / Centro de Ciências Físicas e Matemáticas / Universidade Federal de Santa Catarina

The use of water soluble photoCORM with bioactive ligands can help in directing the CO release from molecular carriers, diminishing the risks of exogenously applied cell signaling gas neurotransmitter

Luminescent Solar Cell Concentrators (LSCs) Based on PMMA Doped with Triplet Dyes: Old Photosensitizers New Perspectives

https://proceedings.science/p/119623

Gianluca Camillo Azzellini [1]; Adrian Kreuz [2]; Gabriel Poplawsky Ciasca [2]; Gustavo Faria Curcio [2]; Elizabeth Grillo Fernandes [3]

[1] Departamento de Química Fundamental / Instituto de Química / Universidade de São Paulo; [2] Universidade de São Paulo; [3] Departamento de Engenharia Metalúrgica e de Materiais / Escola Politécnica / Universidade de São Paulo

PMMA films doped with Ru(bipy)3]2+ or Palladium(II)-Porphyrin display relevant properties for LSCs such as: broad absorption with high absorptivity, large Stoke shifts, and enhanced emission.

Near-infrared fluorescent heptamethine cyanine based scaffolds and their meso substituted derivatives. Photophysics and in vivo imaging

https://proceedings.science/p/120258

Fabiano Severo Rodembusch [1]; Louise Kommers Reimann [1]; Ana Moira Morás [2]; Rodrigo da Costa Duarte [1]; Dinara Jaqueline Moura [2]

[1] Universidade Federal do Rio Grande do Sul; [2] Universidade Federal de Ciências da Saúde de Porto Alegre

Heptamethine cyanines were synthesized in good yields using an innovative methodology and were successfully used as fluorescent probes in biological media, showing a potential for cytoplasm labeling

PHOTO-OMRP of Vinyl Acetate using CoII Complexes Coordinated to New Non-symmetric Schiff Base based on Saloex Systems.

https://proceedings.science/p/119473

Camila Bignardi [1]; Yan Fraga da Silva [1]; Larissa Fazioni de Oliveira [2]; Naralyne Martins Pesqueira [1]; Sergio Murilo Massao Yamada [1]; Beatriz Eleutério Goi [1]; Valdemiro Pereira de Junior [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Departamento de Física, Química e Biologia / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"

The complex [CoIICAYA06] was used to mediate the photo-Organometallic mediated radicalar polymerization of the Vinyl Acetate using TPO as initiator under UV light.

Photocatalytic degradation of organic pollutants via reduced graphene oxide supported on titanium dioxide, and UV-LED mini-photoreactor monitoring

https://proceedings.science/p/120666

Leonardo Zavilenski Fogaça [1]; Jean César Marinozi Vicentini [1]; Camila Fabiano de Freitas [2]; Wilker Caetano [2]; Vagner Roberto Batistela [3]; Mara Heloisa Neves Olsen Scaliante [1]

[1] Universidade Estadual de Maringá / Departamento de Engenharia Química / Programa de Pós-graduação em Engenharia Química; [2] Universidade Estadual de Maringá / Departamento de Química / Programa de Pós-graduação em Química; [3] Universidade Estadual de Maringá / Departamento de Tecnologia / Programa de Pós-graduação em Sustentabilidade

- TEM showed nano-sheets of rGO over the TiO2 anatase crystals with ~120 nm diameter.
- The photodegradations of MB and TAR were 5.7 and 6.9 times faster with the 5rGOTiO2 photocatalyst, respectively

Reversible photoreduction of a phenazine based ligand

https://proceedings.science/p/120686

Lucas Bezerra [1]; Monilson Pinheiro [1]; Idalina M. M. Carvalho [1]; Tércio de Freitas Paulo [2]; Izaura Cirino Nogueira Diogenes [2]; Maria Karolina da Silva Oliveira [3]; João Vitor Ribeiro de Brito [1]

[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica; [3] Universidade Federal do Ceará

Dipyridoquinoxalinophenazine, a highly aromatic chromophore, was synthesized and showed reversible photoreduction reaction upon blue light irradiation

Singlet oxygen generation from a graphene oxide modified with perylene diimide

https://proceedings.science/p/120076

Rayana Martins Peres [1]; Rodrigo Corrêa [1]

[1] Centro de Tecnologia / Universidade Federal do Rio de Janeiro

Electronic energy transfer from graphene oxide to perylene diimide generating reactive oxygen species (ROS) A promissory material for applications in photodynamic therapy

Solvent polarity effect and dual fluorescence behavior of a novel iminochalcone

https://proceedings.science/p/120679

Beatriz Aline Riga Rocha [1]; Miguel Neumann [2]; Carla Cristina S. Cavalheiro [2]
[1] Instituto de Química de São Carlos / Universidade de São Paulo; [2] Universidade de São Paulo

Photophysical properties of a newly synthesized chalcone derivative;
Absorption and emission spectra in different solvents;
Identification of polarity effects and dual fluorescence emission.

Spectroscopic and Computational Methods Applied to Study Photosensitivity and Stability of AmB

https://proceedings.science/p/119785

Gabriel Carvalho de Lima [1]; Marcelo Monteiro Marques [2]; Gláucio Braga Ferreira [1]
[1] Universidade Federal Fluminense - Programa de Pós Graduação em Química; [2] Universidade Federal Fluminense - Colégio Universitário Geraldo Reis

This work is intended to apply strategies to investigate the sensitivity and stability of Amphotericin-B in solid state during exposition to electromagnetic radiation.

Synthesis and photophysical properties of a betalain with potential anti-inflammatory activity

https://proceedings.science/p/119854

Rayani Almeida de Lima [1]; Erick Leite Bastos [2]
[1] Universidade Federal do ABC; [2] Universidade de São Paulo

MefBeet is a fluorescent betalain derived from mefenamic acid and a potential anti-inflammatory drug candidate. Here, we describe the semisynthesis, photophysical and stability properties of mefBeet.

Synthesis of new organometallic complexes of Ni(III) bearing asymmetric Schiff bases to mediate the photoinitiated radical polymerization

https://proceedings.science/p/119488

Naralyne Martins Pesqueira [1]; Larissa Fazioni de Oliveira [2]; Camila Bignardi [1]; Sergio Murilo Massao Yamada [1]; Valdemiro Pereira de Junior [1]; Beatriz Eleutério Goi [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Departamento de Física, Química e Biologia / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"

The syntesis of new complexes of Ni(II) was realized in order to the evaluate the efficiency of Ni (II) complexes in control the photo-OMRP reaction and to obtain the organometallic complex (III).

Synthesis of the [CoII(salen-tert-butyl)] complex coordinated with non-symmetrical Schiff bases to mediate photo-OMRP.

https://proceedings.science/p/119464

Larissa Fazioni de Oliveira [1]; Naralyne Martins Pesqueira [2]; Sergio Murilo Massao Yamada [2]; Camila Bignardi [2]; Valdemiro Pereira de Junior [2]; Beatriz Eleutério Goi [2]
[1] Departamento de Física, Química e Biologia / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Non-symmetrical cobalt(II) [CoII(Salen-tert-butyl)] complex was synthesized in order to mediate the photo-OMRP of vinyl acetate. This complex provided good control in polymerization.

Understanding the photobleaching mechanisms of MEH-PPV

https://proceedings.science/p/119480

Marcelo Gonçalves Vivas [1]
[1] UNIFAL

Produtos Naturais - QPN

1,2,3-triazole derivatives of hydnocarpic acid display antiproliferative activity

https://proceedings.science/p/120730

Marcelo Henrique dos Santos [1]; Liseth Osorio [2]; Guilherme Ferraz [2]; Marisa Ionta [3]; Antonio Demuner [4]; Eduardo Varejão [2]; Guilherme Ferreira [3]; Eduardo Jorge Pilau [5]; Evandro Aparecido Silva [5]; Bianca de Sousa [2]
[1] UFV - Universidade Federal de Viçosa - Campus Viçosa - MG; [2] UFV - Universidade Federal de Viçosa - Campus Viçosa; [3] Universidade Federal de Alfenas; [4] Universidade Federal de Viçosa; [5] Universidade Estadual de Maringá

Antitumor activities of 1,2,3-triazoles from hydnocarpic acid were evaluated. Two of three cell lines tested were inhibited. Hydnocarpic acid may be considered an important prototype for further studi

Absolute configuration of sesquiterpene lactones from Calea pinnatifida

https://proceedings.science/p/120123

Patricia Sartorelli [1]; Andrea N. L Batista [2]; João M. Batista Jr. [3]; João J.H. Lago [4]; Marcelo J. P. Ferreira [5]; Lhaís Caldas [3]
[1] Universidade Federal de São Paulo; [2] Unesp; [3] Unifesp; [4] UFABC; [5] USP

Fractionation of the CH2Cl2 phase of the MeOH extract from the leaves of Calea pinnatifida (Asteraceae) led to the isolation of two related sesquiterpene lactones (STLs): calein C (1) and calealactone B (2). Additionally, during the purification process a derivative of calein C (3) was formed as product of Michael addition of MeOH. The structures of compounds were established based on spectroscopic and spectrometric data [1], while the absolute stereochemistry was established by vibrational circular dichroism for the first time in the literature. VCD associated with density functional theory (DFT) calculations has been demonstrated as a powerful probe to chirality in natural products [2]. The experimental spectra obtained in CDCl3 and simulated data at the B3PW91/6-311G(d,p) level led to the assignment of 4R,6R,7S,8S,9R,10R to compound 1. The most representative vibrational modes used in this assignment were those at (-)-1025 cm-1 (C-O stretch of C-6, C-8, C-9 and C-10), (-)-1125 and (-)-1145 cm-1 (C-H bending of whole molecular framework), as well as (-)-1345 and (-)-1365 cm-1 (out-of-plane and in-plane C-H bending of C-6, C-7, C-8 and C-9). On the other hand, NMR and MS data analysis of (2) demonstrated that this STL is an analogue of (1), containing an epoxide ring at C-2 and C-3. Comparisons of experimental and calculated spectra allowed the assignment of (-)-2 as 2S,3S,4R,6R,7S,8S,9R,10R. As expected, the VCD spectra obtained for (-)-2 were very similar to those of (-)-1 as they share most of the structural and stereochemical features. This is the first report in the literature of the absolute configuration of these sesquiterpene lactones

Alternative low-cost substrates in the production of polyhydroxyalkanoates by isolated strains from D. speciosa

https://proceedings.science/p/120059

Marília Silva Pires [1]; Maria Fatima das Gracas Fernandes Silva [2]; Joao Batista Fernandes [1]; Moacir Forim [1]
[1] Universidade Federal de São Carlos - Departamento de Química; [2] Departamento de Química, Universidade Federal de São Carlos

Bacteria isolated from the insect-pest gastrointestinal tract are capable of producing polyhydroxyalkanoates from different substrates. Use of alternative substrates. Identification of monomeric compo

Antibiotic activities of phomolactone isolated from endophytic fungi co-culture

https://proceedings.science/p/119872

Amanda Gusmão [1]; Elda do Santos [2]; Ivo Caldas [2]; Eliane Silva [1]
[1] UFBA; [2] UNIFAL

(1) Secondary metabolites currently play a crucial role in the search for new lead compounds. Co-culturing of different endophytic fungi rather than maintaining axenic cultures is usually practiced in microbiology to promoting direct interactions that may enhance the accumulation of bioactive secondary metabolites1. As part of our efforts to achieve new bioactive natural products, we carried out the co-culture between two endophytic fungi in the same confined environment. The endophytic strains J1 and J7 had been isolated from Euphorbia umbellata (Pax) Bruyns fresh leaves, which were collected at Vitória da Conquista (Bahia). Mixed and control (axenic) cultures of the fungi were carried out in Petri dishes containing Potato Dextrose Agar (PDA), incubated for 7 days, at 28°C in a B.O.D (Biochemical Oxygen Demand) chamber. After this period, the culture media were extracted with ethyl acetate under sonication. The crude extracts were then analyzed by high-performance liquid chromatography (HPLC). The main secondary metabolites that were biosynthesized by the fungus J1 in axenic cultures were also detected in the co-culture. On the other hand, the biosynthesis of secondary metabolites by J7 was inhibited by the presence of J1. One of the secondary metabolites biosynthesized by the endophyte J1 was isolated and identified as phomalactone (1)2 by NMR and MS techniques (molecular formula C8H11O3 and HRESIMS m/z 155.0708 [M+H+Na]+). The absolute stereochemistry of OH group was determined by optical rotation measurement (+69°, c 0.1, chloroform), and comparison with literature data. Regards the accumulation of compound 1, the amount in the dual culture was almost three times that of axenic culture. Since the biosynthesis of compound 1 was maintained in the endophytic co-culture, we carried out bioassays to access some of its antibiotic activities. The antibacterial activity of 1 was assayed against a panel of pathogenic bacteria: Staphylococcus aureus (ATCC 6538), Escherichia coli (ATCC 8739), and Salmonella enterica (ATCC 6017). The minimum inhibitory concentrations (MICs) were determined by the broth dilution method in 96-well microplates. The compound 1 displayed moderate activity against E. coli and S. enterica MIC = 200 µg/mL. while the reference drug chloramphenicol showed MIC value of 6.25 e 3.125 µg/mL, respectively. Subsequently, the trypanocidal assay was carried out using the Trypanosoma cruzi Y strain. Phomolactone (1) and benznidazole were tested at the same concentrations, in triplicate, for both the trypanocidal and cytotoxicity assays. The IC50 value for 1 against the epimastigote form was 3.12 ± 1.20 µg/mL, while the reference drug benznidazole showed an IC50 value of 8.01 ± 1.31 µg/mL. In the cytotoxicity assay against uninfected H9c2 cells, 1 showed a CC50 value of 37.0 ±1.20 µg/mL, while in comparison the CC50 value for benznidazole was 187.85 ± 2.15 µg/mL. To the best of our knowledge, this is the first time the isolation of the phomolactone (1) from fungi in a co-culture has been reported. This approach efficiently enhanced the yield of this important bioactive compound. Additionally, 1 can act as a chemical signal included in the network established between the endophytes. The very interesting antiparasitic activity of 1 reinforces the pharmacological importance of natural products for which their biosynthesis is activated by microbial interactions. 1Ola, A.R.B.; Daowan Lai, D.T.; BröTz-Oesterhelt, H.; Proksch, P. J. Nat. Prod, 76, 2094−2099, 2013. 2Fukushima, T.; Tanaka, M.; Gohbara, M.; Fujimori, T. Phytochem 48(4):625-630, 1998.

Antinociceptive and Anti-inflammatory Activity of Biomass and Aqueous Extract of Arthrospira platensis Cultivated Indoor

https://proceedings.science/p/119735

Laura Cavalcanti [1]; Guilherme Carneiro Montes [1]; Jeferson Pina Barbosa [2]; Claudia Teixeira [3]; Gisele Zapata-Sudo [1]; Roberto Carlos Campos Martins [1]
[1] Universidade Federal do Rio de Janeiro; [2] SENAI CETIQT; [3] Instituto Nacional de Tecnologia

This work evaluated the antinociceptive and anti-inflammatory activity of biomass and aqueous fraction of microalga A. platensis which is reported to have a broad spectrum of pharmacological activity.

Antioxidant potential of the essential oils of Duguetia echinophora R. E. Fr. and Duguetia riparia Huber (Annonaceae)

https://proceedings.science/p/120709

Angelo Antonio de Moraes [1]; Márcia Moraes Cascaes [2]; Celeste de Jesus Pereira Franco [3]; Giovanna Moraes Siqueira [1]; Lorena Queiroz Almeida [4]; Taina Oliveira dos Anjos [5]; Henryck Fernandes2 [3]; Lidiane Diniz do Nascimento [6]; Pablo Luis Baia Figueiredo [7]; Eloisa Andrade [1]

[1] Laboratório Adolpho Ducke / Coordenação de Botânica / Museu Paraense Emílio Goeldi (MPEG); [2] Programa de Pós-graduação em Química / Universidade Federal do Pará (UFPA); [3] Química Industrial / Instituto de Ciências Exatas e Naturais / Universidade Federal do Pará (UFPA); [4] Engenharia Química / Instituto de Tecnologia / Universidade Federal do Pará (UFPA); [5] Programa de Pós-graduação em Botânica Tropical / Museu Paraense Emílio Goeldi (MPEG) / Universidade Federal Rural da Amazônia (UFRA); [6] Programa de Pós Graduação em Engenharia de Recursos Naturais da Amazônia / Instituto de Tecnologia / Universidade Federal do Pará (UFPA); [7] Departamento de Ciências Naturais / Universidade do Estado do Pará (UEPA)

β-phellandrene and spatulhenol were the major compounds identified in the essential oils of both species. Duguetia echinophora presented a higher capture capacity of DPPH free radicals (38.6% ± 0.68).

Antiparasitic potential against Trypanosoma cruzi of compounds isolated from twigs of Nectandra oppositifolia (Lauraceae)

https://proceedings.science/p/119718

Geanne Conserva [1]; Luis Manoel Quiros Guerreiro [2]; Thais Costa-Silva [1]; Laurence Marcourt [2]; Jean Luc Wolfender [3]; André Gustavo Tempone [4]; Emerson Ferreira Queiroz [2]; João Henrique Ghilardi Lago [5]

[1] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC; [2] University of Geneva; [3] University of Lausanne; [4] Centro de Parasitologia e Micologia / Adolfo Lutz; [5] Universidade Federal do ABC

The EtOH extract from twigs of Nectandra oppositifolia (Lauraceae) displayed anti-Trypanosoma cruzi activity and was subjected to several chromatographic steps to afford three bioactive compounds.

Antitrypanosomal enediyne γ-lactones from fruit peels of Porcelia macrocarpa (Warm.) R. E. Fries (Annonaceae)

https://proceedings.science/p/119877

Fernanda Thevenard dos Santos [1]; Thais Costa-Silva [1]; André Gustavo Tempone [2]; João Henrique Ghilardi Lago [3]

[1] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC; [2] Adolfo Lutz; [3] Universidade Federal do ABC

In this work, the MeOH extract of Porcelia macrocarpa (Warm.) R. E. Fries fruit peels was studied in order to characterize compounds with anti-trypanosomal activity, leading to new enediyne γ-lactones

Antitrypanosomal neolignans from Nectandra reticulata (Lauraceae) twigs

https://proceedings.science/p/120214

Anderson Ueno [1]; Augusto Leonardo dos Santos [2]; Thaís Costa-Silva [3]; André Gustavo Tempone [4]; Patricia Sartorelli [1]; João Henrique Ghilardi Lago [3]

[1] Universidade Federal de São Paulo; [2] UNIFESP Diadema; [3] Universidade Federal do ABC; [4] Adolfo Lutz

The hexane extract from Nectandra reticulata twigs displayed anti-T. cruzi activity and was subjected to bioactivity guided fractionation to afford neolignans acetyl-oleiferin-F 1 and guaicin 2.

Application of computational tools in metabolomics of stingless bee honey

https://proceedings.science/p/119596

Luís Guilherme Pereira Feitosa [1]; Norberto Lopes [2]; Juliana Massimino Feres [3]

[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP) - Universidade de São Paulo/ Departamento de Ciências BioMoleculares (DCBm); [2] Universidade de São Paulo; [3] Heborá

This metabolomic study increased the chemodiversity in stingless bee honeys and opened perspectives to knowledge of potential bioactive compounds and chemical interactions among bees and environment.

Assessment of strategies to activate secondary metabolism of Fusarium oxysporium, an endophyte from Swinglea glutinosa

https://proceedings.science/p/120312

Claudio Yoshio Ogawa [1]; Ana Carvalho [1]; THIAGO VEIGA [1]; Lívia Soman [1]

[1] Universidade Federal de São Paulo

Secondary metabolites produced by microorganisms are an expressive source of bioactive compounds. In particular, endophytic fungi are microorganisms responsible for a great chemical diversity of biomolecules. From Swinglea glutinosa endophytic microbiota, the fungus F. oxysporum was isolated. The specie is responsible for the biosynthesis of beauvericins, a class of molecules that presents several biological activities, such as anticancer, antibacterial and antifungal1. In this sense, this study has seeked the discovery of still unknown beauvaricins analogues, as well as untapped compounds from other classes, applying two different fungal cultivation strategies. The first used different culture media for microorganism growth while the second strategy investigated the metabolic potential of F. oxysporum growing in co-cultures. The preliminary results were obtained through UHPLC-DAD-MS/HRMS based dereplication and molecular networking data analysis (GNPS platform)2. The co-culture with Talaromyces minioluteus, another endophyte from the plant, showed the presence of compounds A (m/z 784) and B (m/z 782) (Figure 2) which showed chemical structure similarities with beauvericins and were not detected in the controls. Molecular networking data analysis also indicated the potential production of A and B analogues. Hominy was highlighted as the best medium regarding potentially new compounds produced by the specie, since it was detected two compounds in this medium, compounds C (m/z 383) and D (m/z 770) (Figure 1). 1. Frontiers in pharmacology 9 (2018):1338. 2. Global Natural Products Social Molecular Networking – http://gnps.ucsd.edu/

Atividade Antiproliferativa de flavonóides diméricos raros, isolados das raízes de Arrabidaea brachypoda

https://proceedings.science/p/120720

Amanda de Jesus Alves Miranda [1]; Carolina Lima [2]; Mayra Cubero [2]; Yollanda Franco [2]; Carla Daniele Pinheiro Rodrigues Rodrigues [1]; Jessyane Rodrigues Nascimento [3]; Débora Barbosa Vendramini Costa [4]; Cláudia Rocha [1]; Giovanna Longato [2]

[1] Universidade Federal do Maranhão; [2] Universidade São Francisco; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [4] Fox Chase Cancer Center

The Cancer is a major concern of the current days. Studies of new compounds with antineoplasic activity, based on natural products, are proving to be increasingly effective in combating this disease.

Atividade citotóxica de triterpenos pentacíclicos isolados de Maytenus quadrangulata (Celastraceae)

https://proceedings.science/p/119802

Mariana Guerra de Aguilar [1]; Grasiely F. de Sousa [1]; Fernanda C. G. Evangelista [2]; Adriano de P. Sabino [2]; Karen Caroline Camargo [3]; Yule R. F. Nunes [4]; Maria O. M. Simões [4]; Lucienir P. Duarte [3]

[1] Departamento de Química, UFMG; [2] Faculdade de Ciências Farmacêuticas, UFMG; [3] Universidade Federal de Minas Gerais; [4] Departamento de Biologia Geral, UNIMONTES

Triterpenos pentacíclicos são comumente encontrados em espécies da família Celastraceae ADDIN ZOTERO_ITEM CSL_CITATION {"citationID":"sfpNEcDv","properties":{"formattedCitation":"(SHAN et al., 2013)","plainCitation":"(SHAN et al., 2013)","noteIndex":0},"citationItems":[{"id":103,"uris":["http://zotero.org/users/4941870/items/BIYJ33BE"],"uri":

["http://zotero.org/users/4941870/items/BIYJ33BE"],"itemData":{"id":103,"type":"article-journal","title":"Natural Friedelanes","container-title":"Chemistry & Biodiversity","page":"1392-1434","volume":"10","issue":"8","source":"Wiley Online Library","abstract":"This review covers the occurrence and biological activities of all natural friedelane triterpenoids found between 1977 and March 2011. The biogeneses of dimeric friedelanes and several rearranged friedelanes are discussed. The pharmacological properties of representative compounds, including celastrol and correolide, have also been compiled, on the basis of 344 references.","DOI":"10.1002/cbdv.201100256","ISSN":"1612-1880","language":"en","author":[{"family":"Shan","given":"Wei-Guang"},{"family":"Zhang","given":"Li-Wen"},{"family":"Xiang","given":"Jia-Gui"},{"family":"Zhan","given":"Zha-Jun"}],"issued":{"date-parts":[["2013",8,1]]}}}],"schema":"https://github.com/citation-style-language/schema/raw/master/csl-citation.json"} , porém poucos compostos isolados de espécies dessa família foram avaliados em relação ao potencial para o tratamento do câncer. Neste trabalho, as folhas de Maytenus quadrangulata (Schrad.) Loes secas e moídas foram submetidas à extração utilizando hexano, clorofórmio, acetato de etila e metanol. Os extratos em hexano e em clorofórmio foram submetidos à purificação por sucessivas cromatografias em coluna, levando ao isolamento de sete triterpenos pentacíclicos: friedelan-3-ona (1), friedelan-3β-ol (2), friedelan-3α-ol (3), friedelan-3,7-diona (4), 3β-hidroxifriedelan-7-ona (5), 3α-hidroxifriedelan-7-ona (6) e 3,4-seco-friedelan-3,11β-olídeo (7). A determinação estrutural dos compostos isolados foi realizada através de métodos espectroscópicos (IV, RMN de 1H e 13C), além da comparação com dados da literatura. A citotoxicidade dos compostos foi avaliada contra as linhagens celulares tumorais humanas THP-1 (células de leucemia mieloide aguda), K562 (células de leucemia mieloide crônica), MDA-MB-231 (células de carcinoma mamário) e TOV-21G (células de carcinoma de ovário). A citotoxicidade dos compostos frente à linhagem Wi-26VA4 (células de fibroblastos de pulmão) foi usada para estabelecer o índice de seletividade. Como controle positivo foram usados os compostos etoposídeo, citarabina e imatinib. Os valores de IC50 bem como o índice de seletividade obtidos estão apresentados na Tabela 1. Todos os compostos testados apresentaram citotoxidade moderada frente às linhagens de células leucêmicas (THP-1, IC50 < 50 µg/mL e K562, IC50 < 80 µg/mL) em comparação com os controles citarabina e imatinibe. Frente a linhagem TOV-21G, os compostos 3, 6 e 7 destacaram-se apresentando valores de IC50 menores que 85 µg/mL e frente a linhagem MDA-MB-231 apenas o composto 3 apresentou citotoxicidade menor que 100 µg/mL. Os compostos apresentaram seletividade superior ou igual ao controle etoposídeo frente a todas as linhagens testadas, porém apresentaram seletividade menor que imatinibe e citarabina, utilizados como controle das linhagens de leucemia. Diante dos resultados observa-se o potencial citotóxico dos triterpenos pentacíclicos isolados das folhas de M. quadrangulata e conclui-se que a continuidade dos estudos da espécie pode contribuir para a obtenção de outros compostos com potencial para o tratamento do câncer.
Agradecimentos CNPq, CAPES, FAPEMIG e Pró-Reitoria de Pesquisa da Universidade Federal de Minas Gerais

Atividade citotóxica e perfil químico do extrato metanólico obtido do caule de Avelós (Euphorbia tirucalli L.) Euphorbiaceae

https://proceedings.science/p/120712

Daniela Cristina Russo [1]; Kleicy Cavalcante Amaral [2]; Lhaís Caldas [3]; Daniel Perez Vieira [2]; Patricia Sartorelli [1]; Waldemar Alves Ribeiro Filho [4]

[1] Universidade Federal de São Paulo; [2] Universidade de São Paulo; [3] Unifesp; [4] Faculdade de Tecnologia de Praia Grande / Centro Estadual de Educação Tecnológica Paula Souza

This phytochemical study carried out with the methanolic extract of Euphorbia tirucalli allowed the identification of phenolic compounds, flavonoids, terpenes and showed cytotoxic potential.

Avaliação antifúngica do óleo essencial in natura das folhas de Cochlospermum regium frente ao desenvolvimento de Rhizopus stolonifer

https://proceedings.science/p/120734

Vinícius Alves do Nascimento [1]; Larissa Liz Sousa Lara [1]; Cássia Cristina Alves [1]; Cristiane Cazal [2]

[1] Instituto Federal de Educação, Ciência e Tecnologia Goiano; [2] Instituto Federal de Educação, Ciência e Tecnologia do Sudeste de Minas Gerais

The essential oil of the leaves of Cochlospermum regium has antifungal activity against Rhizopus stolonifer, a fungus that causes fruit rot.

Avaliação do potencial antiofídico da seiva de Banana Prata (Musa spp.) contra o veneno de Bothrops alternatus

https://proceedings.science/p/120711

Márcia Matos da Silva [1]; Gerso Pereira Alexandre [1]; Lucilia Kato [1]; Ana María Torres [2]; Vanessa Gisele Pasqualotto Severino [1]

[1] Universidade Federal de Goiás; [2] Universidad Nacional del Nordeste

In vitro tests (inhibition of coagulation and hemolysis) were performed to contrast with the results obtained by the SDSPAGE. The species Musa spp. has inhibitory effects against Bothrops alternatus.

Avaliação do teor de óleo essencial de frutos de Schinus molle em diferentes estágios de maturação e localização geográfica

https://proceedings.science/p/120710

Chrystiaine Helena Campos de Matos [1]; Isabela Maria Grossi Leal [1]; Déborah Miranda [1]; Marcelo Henrique Reis Carvalho [1]; Cristiane Cazal [1]

[1] Instituto Federal de Educação, Ciência e Tecnologia do Sudeste de Minas Gerais

Total essential oil content of Schinus molle fruits is significantly affected by the fruits maturation stage, while the tree geographical location had no significant influence.

Avaliação quimiométrica dos semioquímicos produzidos por tomateiros atacados por pragas, utilizando CG-EM.

https://proceedings.science/p/120354

Marcos Henrique Faleiros Santos [1]; Jessica Santos Silva [1]; Marcelo Braga Bueno Guerra [2]; Richele Priscila Severino [3]

[1] Instituto de Química / Universidade Federal de Catalão; [2] Departamento de Química / Universidade Federal de Lavras; [3] Universidade Federal de Catalão

Goiás é o estado brasileiro com maior produção de tomates, no entanto os produtores enfrentam sérios prejuízos econômicos causados pelo ataque de pragas, em especial a mosca-branca (Bemisia tabacci) transmissora do geminivírus. Na tentativa de melhor a produção, empresas têm desenvolvido variedades de tomates resistentes a diversas pragas. Este trabalho objetiva estudar os Compostos Orgânicos Voláteis (VOCs) e Não-Voláteis (CONVs) produzidos por variedades de tomateiros cultivados em Catalão: Dylla (TD) e Norty (TN), sendo TD uma variedade resistente ao geminivírus transmitido pela mosca-branca. Sementes das duas variedades foram germinadas e transplantadas em uma horta particular na cidade de Catalão-GO. Simultaneamente, mudas das mesmas foram cultivadas em uma estufa (controle), na UFCat. Os CONVs foram extraídos das folhas frescas com etanol (extrato etanólico) e os COVs foram coletados usando fibras de microextração em fase sólida (SPME), ambos analisados por Cromatografia Gasosa acoplada a Espectrometria de Massas (CG-EM). Os COVs das variedades cultivadas na estufa foram avaliados por Análise de Componentes Principais (PCA) e PC1, PC2 e PC3 explicam 65,5% da variância. No gráfico de scores a PC1 mostrou a separação dos grupos das duas variedades de tomates (Figura 1A). A análise por SPME apresentou abundância dos compostos: (+)-2-careno, β-felandreno, β-cariofileno, δ-elemeno e humeleno, em ambas as variedades. Notou-se, que TD produziu maior variedade de COVs, entretanto, para os tomateiros cultivados na horta, em contato com a mosca-branca, a variedade TN apresentou aumento na produção de δ-elemeno, β-cariofileno e humeleno. Na análise dos CONVs por PCA, 73,3% da variância entre as duas variedades foi observada pelas PC1, PC2 e PC3. O gráfico de scores, mostrou a variação dos grupos de tomateiros através da PC2 (Figura 1B). A análise dos extratos etanólicos por RMN ^{1}H, mostrou sinais característicos dos compostos identificados por CG-EM, e ainda, sinais na região 6,1-7,0 ppm característicos de compostos aromáticos, sugerindo a presença de ácido salicílico, um composto orgânico associado ao mecanismo de defesa das plantas. Pretende-se realizar novos experimentos de RMN ^{1}H e LC-MS/MS para identificação desses e outros compostos.

Bioprospecting of anti-glycation and antioxidant activities of industrialized pulps and fruit residues

https://proceedings.science/p/120722

Flávia Adaís Rocha dos Santos [1]; Jessika Lane dos Santos Bispo [1]; Felipe Cabral [1]; Lucas Rocha [1]; Júnia Porto [2]; Jadriane de Almeida Xavier [2]; Marília Oliveira Fonseca Goulart [3]

[1] Instituto de Química e Biotecnologia / Universidade Federal de Alagoas; [2] Universidade Federal de Alagoas; [3] Instituto de Química e Biotecnologia (IQB), Universidade Federal de Alagoas (UFAL)

AGEs are related to several chronic diseases. Evaluation of antioxidant and anti-glycation activities of tropical fruits. Fruits have potential for development of antioxidant and anti-AGEs therapies.

Biossensor Eletroquímico de Acetilcolinesterase aplicado para substâncias naturais inseticidas

https://proceedings.science/p/120738

Sean dos Santos Araújo [1]; Joao Batista Fernandes [1]; Ronaldo Farias [1]; Wilson Tiago da Fonseca [1]

[1] Universidade Federal de São Carlos

The present work aims to immobilize the enzyme acetylcholinesterase (AChE) in SPEs (Screen-Printed Electrode) for inhibition assays. The azadiractin, showed significant inhibition in this assay.

Caramboxin tissue distribution in Star Fruit

https://proceedings.science/p/119629

Pâmela Rodrigues Rosa Pereira [1]; Jacqueline Nakau Mendonça [1]; Norberto Lopes [2]

[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP); [2] Universidade de São Paulo

Highlights: Caramboxin concentration is higher in the seeds and surrounding areas. In recent years, some studies have demonstrated several cases of star fruit (Averrhoa carambola) intoxication in patients with chronic kidney disease (CKD), since then its has sought to know the cause of these effects. In 2013, Garcia-Cairasco and collaborators identified and characterized the compound responsible for triggering this intoxication and called it caramboxin (CBX). However, the caramboxin distribution in the fruit was still unknown, due to the fact that the researchers isolated this toxin from the whole fruit, without separating the different parts. Thus, this study aimed to identify the caramboxin tissue distribution in star fruit. Star fruits were collected Ribeirão Preto downtown - São Paulo, sectioned crosswise in cryostat and the slices transferred immediately to a conductive glass plate specific for MALDI-imaging (Bruker Daltonics®), then a suspension of inorganic titanium dioxide matrix in water:acetonitrile was sprayed. The plate covered with matrix was inserted in the MALDI-TOF/TOF Ultraflextreme equipment, the analyzes were performed and the data were treated generating the images, using the SCLIS® software. The images obtained show that caramboxin is concentrated in the seeds and surrounding areas. Knowledge of the caramboxin tissue distribution may be relevant in the investigation of its biosynthetic origin, beyond to contributing to doctors and nutritionists in guiding patients that are at risk groups for star fruit intoxication.

Cellulose acetate-based membranes from the banana pseudostem containing extracts the fruit of Butia catarinensis

https://proceedings.science/p/119570

Rachel Faverzani Magnago [1]; Nathan R. L. Pereira [1]; Bruna Lopes Lopes [1]

[1] Universidade do Sul de Santa Catarina (UNISUL)

Extracts from the fruit of Butia were obtained and incorporated into the cellulose of the banana pseudostem membranes. Thermal stability was maintained and mechanical strength was improved.

Chemical characterization and anti-inflammatory activity of Siparuna guianensis Aublet leaves

https://proceedings.science/p/119681

Jéssica L. M. Conegundes [1]; Josiane M. da Silva [2]; Renata F. Mendes [1]; Paula R. B. Dib [3]; Gilson C. Macedo [3]; Elita Scio [4]
[1] Universidade Federal de Juiz de Fora/Departamento de Bioquímica; [2] Universidade Federal de Juiz de Fora/Departamento de Bioquímica; [3] Universidade Federal de Juiz de Fora/Departamento de Parasitologia, Microbiologia e imunologia; [4] Universidade Federal de Juiz de Fora

The leaves of Siparuna guianensis Aublet, known as negramina, are used by indigenous and local communities in Brazil and other American countries to treat pain and inflammatory disorders 1. Thus, this study aims to characterize the chemical constituents and to evaluate the in vitro and in vivo anti-inflammatory activity of the dichloromethane fraction of S. guianensis leaves. The chromatographic profile was determined by Ultra Performance Liquid Chromatography - Mass Spectrometry (UPLC-MS), and the study of the anti-inflammatory activity was carried out by nitric oxide (NO) measurement in LPS-stimulated macrophages (J774.A1 cell line) 2 and by croton oil-induced ear edema assay, in mice 3. A mixture of glycosylated and methoxylated flavonoids was tentatively characterized by the UPLC-MS technique. In protonated mode, kaempferol-pentosyl-pentoside-rhamnoside (m/z 697) and kaempferol-di-rhamnoside (m/z 579) were identified. In deprotonated mode, the presence of kaempferol-pentosyl-rhamnoside (m/z 563), rhamnosyl-kaempferol (m/z 431) and kaempferol dimethylether (m/z 313) was observed 4. Concerning to the anti-inflammatory activity, the DF (50 to 5 µg/mL), when compared to the LPS+IFN-γ stimulated group, was able to reduce the NO production in 80%, 42% and 24% at doses 50, 25, and 10 µg/mL, respectively in J774.A1 macrophages. DF reduced significantly the mice ear edema induced by croton oil at 100, 200 and 300 mg/kg in 54%, 30%, and 53%, respectively. This result is quite interesting, as no statistical difference was found when compared to indomethacin (45% of inhibition). The ear edema assay is widely used and it is recognized as a useful pharmacological model for the investigation of new drugs of plant and synthetic origin with anti-inflammatory activity. The presence of glycosylates flavonols and kaempferol dimethylether in DF may be related to the activities found 5,6. In conclusion, those results emphasized the anti-inflammatory activity of S. guianensis, supporting the ethnopharmacological use of this species

Chemical characterization by molecular networking prospection and antinociceptive activity of Croton antisyphiliticus (Euphorbiaceae)

https://proceedings.science/p/120109

Stephanie Prado [1]; Gerso Pereira de Alexandre [2]; Núbia A. M. T. P. Gomides [3]; Dionys de S. Almeida [1]; Aline N. Martins [1]; Daiany P. B. da Silva [1]; Elson A. Costa [1]; Vanessa Gisele Pasqualotto Severino [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal de Goiás; [3] Universidade Federal de Catalão

Croton is the second largest genus of the family Euphorbiaceae. The species C. antisyphiliticus Mart., from Cerrado biome, is popularly known as pé-de-perdiz and widely used in folk medicine due to its therapeutic properties. The aqueous root extract of this species is popularly used for sexually transmitted infections, diseases of the reproductive system, colic treatment, rheumatism, against fungi, ulcer wounds and inflammation. In this work, an ethnobotanical study was carried out in the Coqueiros community, located in Catalão, Goiás state, and C. antisyphiliticus was mentioned to antibiotic, infection of the uterus and influenza. This information instigated the chemical and anti-inflammatory studies of the ethanolic and aqueous extracts from roots to verify and better elucidate therapeutic effects of these. The roots of C. antisyphiliticus were identified and collected; the testimony species is deposited in the Herbarium of the Federal University of Goiás, under the code UFG-27,850, as well as registered in the SisGen under the code A11AE20. Preparation of crude extracts of the roots occurred by two methodologies: 1. following the Coqueiros community method boiling the fresh roots in water and freeze-drying the solvent, obtaining the aqueous root extract (EAR); 2. extraction of the dried roots with ethanol for nine days (exchange every three days), followed by evaporation of the solvent in rotary evaporator, low pressure, obtaining the ethanolic extract of the roots (EER). The chemical characterization of extracts was performed by liquid chromatography–mass spectrometry (LC-MS) using a Thermo Scientific Q Exactive Focus LC-MS/MS equipment coupled to a UHPLC Dionex UltiMate 3000 and data were analyzed using GNPS platform and Cytoscape software to obtain molecular networks. The antinociceptive activity of extracts was evaluated in the Irwin test, acetic acid-induced writhing test, formalin-induced pain test and tail flick test. The chemical characterization revealed the presence of phenolic compounds in both the extracts. Gallic acid, protocatechuic acid, catechin, epicatechin, gentisic acid, luteolin and kaempferol were identified in the EER; and epicatechin, gentisic acid and caffeic acid in EAR. In addition, by the dereplication using GNPS platform was identified L-gulonolactone in EER and also gallic acid, protocatechuic acid, ellagic acid and catechin compounds. In Irwin test, EER [doses of 125, 250 and 500 mg kg-1 (p.o.)] and EAR [doses of 300, 600, 900, 1200 or 1500 mg kg-1 (p.o.)] were determined to be used in subsequent pharmacological tests. The treatment with EER [125, 250 and 500 mg kg-1 (p.o.)] reduced the number of writhing in a dose-dependent manner by 30, 53 and 41%, respectively, when compared to the vehicle group. In formalin-induced pain, EER [250 mg kg-1 (p.o.)] decreased the licking time in the first and second

phase by 36 and 31%, respectively, when compared to the vehicle group. However, this same dose of EER did not cause effect in tail flick test. Treatment with EAR at doses and 600, 900, 1200 or 1500 mg kg-1 (p.o.) reduced the number of writhing by 14, 25, 44 and 44%, respectively, compared to the vehicle group. These results showed significant antinociceptive effect of EER and EAR, which may be associate to the presence of phenolic compounds identified in both the extracts, since the antinociceptive and anti-inflammatory activities of these constituents are described in the literature. In conclusion, the present study suggests an antinociceptive activity of EER and EAR from C. antisyphiliticus, which may be association to presence of phenolic compounds. However, further studies are needed to investigate the mechanisms of action involved in this effect.

Chemical composition and acaricidal effect of essential oils of Croton species on larvae of Rhipicephallus microplus.

https://proceedings.science/p/119453

Geovany Amorim Gomes [1]; Felipe F. da Silva [1]; Susy das G. A. Alves [2]; Maria Geysillene C. Matos [3]; Francisca Letícia V. da Silva [2]; Paula B. Cruz [4]; Tigressa H. S. Rodrigues [1]; Elnatan B. de Souza [1]; Caio Márcio de O. Monteiro [2]
[1] Universidade Estadual Vale do Acaraú; [2] Universidade Federal de Goiás ; [3] Universidade Regional do Cariri ; [4] Universidade Federal de Juiz de Fora
Os óleos essenciais de plantas têm sido investigados na busca do desenvolvimento de novos agentes ativos contra carrapatos, pois, ao contrario dos acaricidas sintéticos, são mais seletivos e menos agressivos ao homem e ambiente. Com 68 espécies difundidas na flora do Nordeste brasileiro, principalmente na região de Caatinga, plantas do gênero Croton (Euphorbiaceae) são utilizadas pela população para tratar diversas enfermidades e são produtoras de óleos essenciais, ricos em fenilpropanoides, mono e sesquiterpenoides, com eficácia comprovada contra o carrapato Rhipicephalus microplus. Assim, o objetivo deste trabalho foi caracterizar quimicamente e avaliar a atividade acaricida dos óleos essenciais de C. grewioides (EOCG) e de C. virgultosus (EOCV) frente ao carrapato R. microplus. Os óleos foram obtidos a partir da hidrodestilação de folhas de cada espécie durante 2h, com rendimento de 2,11% (w/w) para EOCG e 0,45% (w/w) para EOCV. As análises químicas realizadas em CG/EM e GC/DIC levaram a identificação de 13 constituintes no EOCG, totalizando 99,63% desse óleo, apresentando como componente majoritário o anetol (88,95%). Enquanto que em EOCV foram identificados 23 constituintes, representando 98,59% de sua composição, sendo metil eugenol (49,25%) e 1,8-cineol (13,26%) seus constituintes mais abundantes. Para avaliar a eficácia dos óleos, realizou-se o teste de pacote de larvas. Os resultados revelaram que EOCG e EOCV, óleos ricos em fenilpropanoides, exibiram ação biocida frente a R. microplus (CL50 = 3,57 e 4,78, respectivamente) e são promissores para o desenvolvimento de novos acaricidas.

Chemical composition and antimicrobial activity of the essential oil from Croton urticifolius

https://proceedings.science/p/120150

Maria da Conceição de Menezes Torres [1]; Antonio Junior Costa Barbosa [1]; Havana Lorena S. de Araujo [1]; Mateus A. da Luz [1]; Maisa Fernanda dos S. Barbosa [2]; Bruno O. Veras [2]; Marcia Vanusa da Silva [2]
[1] UEPB; [2] UFPE
O gênero *Croton*, um dos maiores da família Euphorbiaceae, possui espécies aromáticas que produzem óleos essenciais ricos em monoterpenos, sesquiterpenos e fenilpropanóides. Os óleos essenciais de Croton são conhecidos por apresentarem atividades biológicas, tais como anti-inflamatório, antioxidante, antimicrobiana, citotóxico, entre outras.1-2 O objetivo deste trabalho foi investigar a composição química e a atividade antibacteriana do óleo essencial das folhas de Croton urticifolius do brejo paraibano. As folhas frescas (1 kg) de C. urticifolius foram extraídas por hidrodestilação em aparelho de Clevenger por 3 hs. O óleo essencial foi analisado por CG/EM para identificar a composição química. A análise CG/EM permitiu a identificação de 19 compostos (96,0%) e os principais compostos foram: α-pineno (21,70%; 1), 2. biciclogermacreno (21,46%) e 3. (E)-cariofileno (17,34%) (Fig. 1). A atividade antibacteriana foi testada frente às cepas de Escherichia coli (ATCC 8739) e Staphylococcus aureus (ATCC 6538). O óleo apresentou atividade antibacteriana apenas frente à E. coli, com concentração inibitória mínima (CIM) de 512 µg mL-1. Este valor é considerado uma inibição forte,3 demonstrando que este óleo pode servir de base para a formulação de novos agentes antimicrobianos. No entanto, são necessários estudos in vivo para a avaliação de possíveis mecanismos bioquímicos subjacentes.

Chemical study of Fusarium solani, an endophyte fungal strain isolated from the red marine alga Dichotomaria marginata

https://proceedings.science/p/119895

Edelson de Jesus Sá Dias [1]; Alana Evangelista Honório [1]; Dulce Helena Siqueira Silva [1]; Givaldo Silva [1]; Ana Letícia Pires dos Santos [1]; Letícia Cristina Vieira Atanázio [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Isolation of endophytic fungus Fusarium solani from the marine red alga Dichotomaria marginata, identification of low molecular weight phenolic acids by GC-MS. The bioassays evidenced antileishmania and cytotoxic potential of the crude extract.

Chemical study of Penicillium sp. (AcR02), endophyte of Rhizophora mangle

https://proceedings.science/p/120087

Patrícia Marinho [1]; Gisele da Costa Ramos [1]; Lyandra Cristina Ferreira Pereira [1]; Luciano Almeida Watanabe [1]; Andrey Moacir do Rosario Marinho [1]

[1] Universidade Federal do Pará

The present work reports six substances produced by the fungus Penicillium sp. (AcR02), endophyte of Rhizophora mangle, from Village of the Acarajó, Bragança-PA.

Chromatographic profile as a tool for the chemical study of Brazilian cultivated plants

https://proceedings.science/p/120750

Valéria Regina de Moraes [1]

[1] Universidade Federal de Sergipe

Composição de voláteis do mel de Apis mellifera e Melipona subnitida

https://proceedings.science/p/120723

Adriana Flach [1]; Edineide Cristina Alexandre de Souza [1]; Sílvio José Reis da Silva [2]

[1] Universidade Federal de Roraima; [2] MUSEU INTEGRADO DE RORAIMA

Volatile composition from Apis mellifera and Melipona subnitida honeys
Melipona subnitida has honey with esters as predominant components
Apis mellifera honey has complex composition

Composition of Essential Oil from Inflorescences of Magonia pubescens A.St.-Hil.

https://proceedings.science/p/120707

Acácio Raphael Moraes [1]; Grasiely Sousa [2]; Maria Simões [3]; Márcio Pereira [4]; Lucienir Duarte [1]; Antônio Alcântara [1]

[1] Universidade Federal de Minas Gerais; [2] Departamento de Química, UFMG; [3] Universidade Estadual de Montes Claros; [4] Centro de Desenvolvimento da Tecnologia Nuclear

The composition of essential oils from Magonia pubescens were obtained by hydrodistillation. Hotrienol, cis-linalool oxide, and trans-linalool oxide were identified as the main components.

Compostos fenólicos e extrato antioxidante e aleloquímico do fungo endofítico Coriolopsis rígida isolado de Cochlospermum regium

https://proceedings.science/p/119766

Vanessa Chapla [1]; Sara Dantas [1]; Angela Araujo [2]
[1] Universidade Federal do Tocantins; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"

First report of phenolic compounds from Coriolopsis rigida.
Antioxidant Activity for Coriolopsis rigida crude extract.
Endophyte Coriolopsis rigida isolated from medicinal plant of the Cerrado.

Compounds isolated from the leaves of Stizophyllum perforatum

https://proceedings.science/p/119834

Osvaine Alves [1]
[1] Universidade de Franca

The Stizophyllum perforatum leaves extract and hexane fraction showed leishmanicidal activity. The hexane fraction was purified by chromatographic column, and yielding triterpene and steroids.

Compounds isolated in the EtOAc fraction from Paepalanthus acanthophyllus (Eriocaulaceae)

https://proceedings.science/p/120717

Laysa Lanes Pereira Ferreira Moreira [1]; Raphael Conti [1]; Warley Borges [1]; Lucas A. Oliveira
[1] Universidade Federal do Espírito Santo

Novel compounds were isolated in the ethyl acetate fraction from Paepalanthus acanthophyllus (Eriocaulaceae) by classical e modern chromatography techniques.

Cytochalasin derivatives from Diaporthe sp., an endophyte isolated from leaves of Casearia arborea (Salicaceae)

https://proceedings.science/p/119714

Augusto Leonardo dos Santos [1]; Eunizinis dos Santos Kawafune [2]; Renato O. Horvath [3]; Marisa Ionta [4]; Marisi G. Soares [4]; Marcelo J. P. Ferreira [2]; Patricia Sartorelli [5]
[1] UNIFESP Diadema; [2] USP; [3] Universidade de São Paulo; [4] UNIFAL; [5] UNIFESP
Diaporthe spp. has diverse host associations, frequently found as endophyte in plants. Its special metabolites present a broad range of biogenesis origin, including a great diversity of polyketides, as well terpenoids, alkaloids and peptides. About 66% of secondary metabolites are related to microorganisms found in plants and 84% of secondary metabolites from microorganisms are related to fungus. Endophytes found in Casearia are restricted, so the bioprospection of endophytic fungi from leaves of C. arborea was done according to literature[5] and the cytotoxic activity screening showed the cellular viability of 40% for A549 (human lung carcinoma) and HT144 (human melanoma), and 60% for MCF-7 (human breast cancer) in presence of EtOAc extract from CarGL-08 strain cultivated in rice. The fungi identification was based on molecular approach and sequencing of ITS region. CarGL08 strain belongs to Diaporthe sp. genus (Phomopsis-like) and through. Fractionation of its polar phase an alkaloid was isolated and identified as cytochalasin H by ^{1}H and ^{13}C NMR, UV and MS/MS spectra. From this compound, the analysis of GNPS-molecular networking[7] showed the presence of cytochalasin D (figure 1) and analogues in the process of identification by MS/MS fragment analysis.

Design of Experiments applied to the analyses of soy by-products

https://proceedings.science/p/120739

Felipe Sanchez Bragagnolo [1]; Márcia Cristina Breitkreitz [2]; Cristiano Soleo Funari [3]

[1] Departamento de Bioprocessos e Biotecnologia / Faculdade de Ciências Agronômicas / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual de Campinas; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"

- Agricultural by-products can be a source of high-added value compounds - Soybean is the main Brazilian commodity - Design of experiments (DoE) approach should be preferred over a "trial-and-error" a

Determinação do perfil fitoquímico e avaliação comparativa da atividade antioxidante do extrato etanólico e frações, das flores da espécie Hibiscus sabdariffa L.

https://proceedings.science/p/120731

Marlene Santos da Silva [1]; Katyuscya Leao [1]

[1] Universidade Federal do Oeste da Bahia

Phytochemical study and comparative analysis of data obtained for antioxidant activity by the DPPH and ABTS methods of extract and fractions obtained from dried flowers of the species H. sabdariffa

Determinação dos ácidos caféico e p-cumárico em extratos comerciais de própolis por CLAE-DAD após separação por EFS.

https://proceedings.science/p/120703

Daniela Lemos Cavalcante Guedes Machado [1]; Isabela de Paula Lima [2]; Christiane Duyck [3]; Raquel Andrade Donagemma [3]; Fernando Antonio Simas Vaz [3]

[1] Universidade Federal Fluminense; [2] Instituto de Química / Programa de Pós-Graduação em Química, UFF; [3] Instituto de Química / Departamento de Química Analítica, UFF

Caffeic and p-coumaric acids were determined in commercial propolis extracts. Antioxidant activity and polyphenols amounts in the samples were compared to the concentrations of these acids.

Determination of phenolic compounds in aqueous phase from pyrolysis of guava seeds using LC-DAD and biological evaluation.

https://proceedings.science/p/120100

Valéria Regina de Moraes [1]; Júlio Oliveira [1]; Lisiane dos Santos Freitas [2]; Antonia Regina dos Santos Gois [1]; Vilma Prado [1]; Raphael Amancio de Jesus [1]; Pedro Ellison Santos do Nascimento [1]; Jussara Oliveira Santos [1]; James Silva [1]; Rafael Ciro Marques Cavalcante [1]

[1] Universidade Federal de Sergipe; [2] Universidade Federal de Sergipe, Departamento de Química

Four phenolic derivatives were identified in the aqueous phase produced from pyrolisis of guava seeds. Catechol was the major compound. The aqueous phase showed potent antioxidant activity.

Determination of total phenols and antioxidant in tomato, strawberry, and coffee using smartphone

https://proceedings.science/p/120704

Cristiane Isaac Cerceau [1]; Edmar J. O. Bazani [1]; Matheus S. Barreto [1]; Antonio Demuner [1]; Marcelo Henrique dos Santos [1]; Daiane Einhardt Blank [2]; Maria Firmino [1]; Gustavo Souza [1]

[1] Universidade Federal de Viçosa / Departamento de Química; [2] Universidade Federal de Viçosa

A simple and fast method for determination of total phenols and antioxidant in tomato, strawberry, and coffee was developed. It can be carried out using a smartphone camera and a portable apparatus.

Diaporthe phaseolorum molecular family analysis using GNPS platform

https://proceedings.science/p/120052

Mariana Moura [1]; Jhuly W. F. Lacerda [1]; Arielly C. R. dos Santos [2]; Marcos A. Soares [2]; Paulo T. de Sousa Jr [2]; Evandro Dall'Oglio [2]; Lucas C. C. Vieira [2]; Olívia M. Sampaio [2]

[1] Universidade Federal de Mato Grosso (UFMT); [2] UNIVERSIDADE FEDERAL DE MATO GROSSO

Natural products are an important source of bioactive compounds discovery. Thesecompounds played a relevantrole onbiotechnologydevelopment, as medicine prototypes, in the fungi and bacteria controland usedas allelochemicals to plant growthinhibition.1,2Due to the importance of natural products, new computational approaches to chemical interpretation of large data sets have been develop, such as molecular networks, which is a molecular mining tool to findmolecular families and substructures in mass spectrometry fragmentation data.3,4Despite these advances, interpreting large-scale, non-targeted metabolomic datasetis still a challenge when reference spectra are not available or when chemical structures need to be assigned.4Thus, in order to improvechemical structural information in a molecular network, the MolNetEnhacer tool (https://ccms-ucsd.github.io/GNPSDocumentation/molnetenhancer/)was implemented on the GNPS platform (Global Natural Products Social Molecular Networking), which accelerates the chemical structural annotation in complex mixtures through the combined use of networks spectral molecular masses, fragmentation patterns and in silicoannotations, providinga more comprehensive chemical overview of spectral data.4This tool is based on the molecular structure similarity (analogs) which generate fragmentation spectra that can be grouped according to the chemical classes presentin the biological sample.4The chemical classesknowledge of secondary metabolites present in an extract increases the ability to supply mechanistic explanations for the biological behavior of the matrix (structure / activity relationship), in addition toenabling a prior analysis of whether the matrix will answer the proposed research hypotsis.3,4Therefore, in this work, the MolNetEnhacer tool was employedto track and identify the chemical classes contained in Diaporthe phaseolorum(Dp)ethyl acetate extract, which has biological potential already described in the literature as bioherbicide, antioxidant, antimicrobial, antifungal, antibactericide, antitumor and larvicide1,5,6,using LC/Q-TOF-MS/MS and the GNPS platform (http://gnps.ucsd.edu).There were identified 109compounds of11 chemical classes in the network using MolNetEnhancer, where molecular families are mainly describedas carboxylic acids and derivatives, fatty acids, flavonoids, homoisoflavonoids, indoles and derivatives, organooxygen compounds, piperidines, prenol lipids, nucleosides of purine, azoles,steroids and derivatives. Based on these results, we conclude that MolNetEnhancer is anuseful tool that greatly helps the researcher allowing prior knowledge of the chemical characteristics of the matrix of interest.

Entendendo a comunicação química entre os simbiontes das formigas cortadeiras usando análise multivariada e mapas moleculares

https://proceedings.science/p/120713

Alana Kelyene Pereira [1]; Dorai Zandonai [1]; Anelize Bauermeister [2]; Joao Batista Fernandes [1]

[1] Universidade Federal de São Carlos; [2] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP)

Different approaches such as molecular networking and multivariate analysis can help to understand the chemical interactions among leaf-cutting ants symbiont microbes.

Estudo da atividade leishmanicida de plantas do cerrado utilizando arginase como alvo biológico.

https://proceedings.science/p/120735

Matheus Barros [1]; Eduarda Oliveira [2]; Romário Pereira da Costa [3]; Quezia Bezerra Cass [3]; Dulce Helena Ferreira de Souza [3]; Lorena Ramos Freitas de Sousa [4]; Richele Priscila Severino [2]

[1] Universidade Federal de Uberlândia; [2] Universidade Federal de Catalão; [3] Universidade Federal de São Carlos; [4] Universidade Federal de Goiás

This work consisted of the screening of natural products extracts against arginase. From the leaves extract of Byrsonima coccolobifolia (Malpighiaceae) 12 ligands were identified and 9 characterized.

Estudo fitoquímico das folhas de Schinus Terebinthifolius Raddi

https://proceedings.science/p/120032

Jean Lucas Silva de Almeida [1]; Eliezer Silva [1]; Jorge David [2]; Rodrigo de Paula [1]

[1] Universidade Federal do Recôncavo da Bahia; [2] Universidade Federal da Bahia

Schinus Terebinthifolius Raddi is a pepper plant that has antifungal, antioxidant and antimicrobial properties. The chemical profile of its leaves is described in this work.

Estudo fitoquímico do extrato hexânico das folhas de Pristimera celastroides (Celastraceae)

https://proceedings.science/p/119794

Karen Caroline Camargo [1]; Lucienir Pains Duarte [1]; Grasiely Faria de Sousa [1]; Raquel Goes de Castro [1]; Mariana Guerra de Aguilar [1]

[1] Universidade Federal de Minas Gerais

A espécie Pristimera celastroides, pertencente à família Celastraceae, é uma liana encontrada em áreas florestadas. Na medicina popular é usada no tratamento de infecções, inflamações e doenças gástricas.1 Neste trabalho, as folhas secas e moídas de P. celastroides foram submetidas a extração exaustiva por maceração utilizando os solventes hexano, clorofórmio e metanol. O extrato hexânico foi fracionado por sucessivas cromatografias em coluna, resultando na purificação de sete compostos: esqualeno (1), 3β-aciloxi-9,19-ciclolanost-24-ene (2), guta-percha (3), α-tocoferol (4), β-sitosterol na sua forma esterificada (3β-aciloxi-sitosterol; 5) e livre (6) e 3β-aciloxi-9,19-ciclolanost-24,25-diol (7). Esses foram identificados a partir da análise dos espectros de RMN de 1H, 13C e DEPT-135, bem como pela comparação com dados da literatura. Todos os compostos isolados são relatados pela primeira vez para P. celastroides, e os compostos da classe dos cicloartanos, 2 e 7, são inéditos na família Celastraceae.

Estudo químico e fitotóxico do extrato hidroetanólico das folhas de Machaerium amplum Benth.

https://proceedings.science/p/121400

Luciana Sayuri Tahira [1]; Marcelo Marucci Pereira Tangerina [2]; Renan Canute Kamikawachi [3]; Priscila Torres [2]; Marcelo J. P. Ferreira [4]; Ângela Lúcia Bagnatori Sartori [5]; Wagner Vilegas [3]; Miriam Sannomiya [1]

[1] Escola de Artes, Ciências e Humanidades / Universidade de São Paulo; [2] Instituto de Biociências / Universidade de São Paulo; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [4] Universidade de São Paulo; [5] Universidade Federal de Mato Grosso do Sul - Campo Grande

Chemical and phytotoxic study of the hydroethanolic extract of the leaves of Machaerium amplum Benth. The chemical study by FIA-ESI-IT-MS and HPLC-ESI-MS of M. amplum extract furnish the identificatio

EUGENILLA ACETATE PRODUCTION FROM Syzygium aromaticum ESSENTIAL OIL BIOCATALIZED BY THE ENDOPHYTIC FUNGUS Sordaria sp.

https://proceedings.science/p/119739

Maíra Marini [1]; Maria Sandra Queiroz [2]; Rogério Dallago [3]; Natalia Paroul [4]; Leopoldo Clemente Baratto [1]; Ivana Correa Ramos Leal [1]; Michelle Frazão Muzitano [1]

[1] Universidade Federal do Rio de Janeiro; [2] Universidade Federal de Juiz de Fora; [3] Universidade Regional Integrada do Alto Uruguai e das Missões; [4] Universidade Regional Integrada do Alto Uruguai e das Missões – Campus Erechim, Departamento de Química

Os óleos essenciais são misturas de substâncias voláteis, lipofílicas, geralmente odoríferas e líquidas,compostas por mais de 300 componentes químicos diferentes, entre eles terpenos e fenilpropanoides, fazendo deles um produto de importância industrial(Wolffenbüttel, 2007). Há basicamente três métodos para se obter substânciasde aroma: extração direta da natureza, transformações químicas ou transformações por via biotecnológica (Franco, 2004). Além de serem menos agressivos ao meio ambiente, os processos biotecnológicos produzem aromas considerados naturais (Janssens et al., 1992). O sistema livre de solventes, além do uso de biocatalisador imobilizado, facilita os processos de purificação,promove uma redução de custos e possibilita o uso de altas concentrações de substratos (Güvens et al., 2002).O objetivo desse trabalho foi verificar a produção do acetato de eugenila a partir do óleo essencial de cravo da índia - OECI (Syzygium aromaticum)em sistema livre de solvente orgânico, utilizando como biocatalizador o extrato bruto enzimático imobilizado em poliuretano do fungo Sordariasp. (TB1).O perfil cromatográfico do OECIfoirealizado por meio de cromatografia gasosa acoplada à espectrometria de massas (CG-EM) em equipamento Shimadzu GC-MS

2010, comcoluna Quadrex 007-5MS (30 m x 0,025 µm);temperatura inicial de 60°C, elevando até 260°C numa razão de 3°C/min, permanecendo nesta temperatura durante 10 min;gás de arraste: hélio (59 kPa) e Split1/10. O tempo da análise foi de72 min. Para a esterificação do OECI,foram utilizados 3,41g de óleo essencial; 7,51g de anidrido acético e 1g do extrato bruto enzimático de TB1, obtido após ensaios de precipitação do seu cultivo, imobilizado em espuma de poliuretano,queconsiste na reação entre monômero poliol poliéter (5 mL = 50 %)eisocinato (tolueno diisocianato - TDI) (5 mL = 50 %),poraté 8h, à 60°C, 180 rpm (Shaker). A análise do OECI apresentou o eugenol (biblioteca NIST 05) como constituinte majoritário, com área relativa de 63,3% e tempo de retenção de 19,32 min. A determinação do percentual de conversão ao acetato de eugenila foi realizadamonitorandopor CG-EM, a cada 1h, a redução da área integrada do sinal referente ao agente limitante (eugenol)no OECI,em comparação ao OECI esterificado.No tempo de 5 h foi possível observar 55,9% de esterificação, enquanto que ao final do tempo reacional foi possível verificar 72,55% de esterificação do eugenol. Vain (2014) descreveu a esterificação do eugenol no OECIde 99,87% nas mesmas condições utilizadas neste trabalho,entretanto, com a enzima comercial Novozym 435,o que torna nossos dados ainda mais promissores, considerando que focamos no uso de um extrato bruto enzimático imobilizado.Mais estudos precisam ser realizados afim de determinar a cinética da reação e a aplicabilidade do extrato bruto enzimático em outras reações de esterificação de produtos de aroma, bem como o reciclo do biocatalisador nas reações de sucesso.

Evaluation of the antiparasitic activity of isolated metabolites from aerial parts of Hydrocotyle bonariensis Lam. (Araliaceae)

https://proceedings.science/p/119797

Dalete Christine da Silva Souza [1]; Thais Costa-Silva [2]; André Gustavo Tempone [3]; João Henrique Ghilardi Lago [2]
[1] Federal University of São Paulo / Institute of Environmental, Chemical and Pharmaceutical Sciences; [2] Federal University of ABC / Center of Natural and Human Sciences; [3] Adolfo Lutz Institute / Center for Parasitology and Mycology

This work seeks to isolation/characterization of bioactive compounds from Hydrocotyle bonariensis and evaluation of activity against the parasites Trypanosoma cruzi and Leishmania infantum.

Exploration of Trichoderma spirale chemical classes employing GNPS

https://proceedings.science/p/120028

Arielly Celestino Rodrigues Santos [1]; Mariana Moura [1]; Jhuly W. F. Lacerda [1]; Marcos A. Soares [1]; Evandro L. Dall'Oglio [1]; Lucas C. C. Vieira [1]; Paulo T. Sousa Jr [1]; Olívia M. Sampaio [1]
[1] Universidade Federal de Mato Grosso (UFMT)

Mass spectrometry is a technique used to identify compounds in undirected metabolomics experiments. Due to the reference spectra absence, most molecules cannot be identified and many spectra cannot be used. In this context, the MolNetEnhacer (https://ccms- ucsd.github.io/GNPSDocumentation/molnetenhancer/), a method that was implemented on the GNPS platform (http://gnps.ucsd.edu), to accelerate the chemical structural annotation in complex matrix combining mass spectral molecular networks, fragmentation patterns and in silico annotations, providing a more comprehensive chemical overview of spectral data. This tool allows analysing the chemical classes and subclasses in the molecular networking. Based on the predominant chemical classes present in a plant extract, significantly increases the ability to provide explanations for the matrix biological behaviour, as well as assessing whether molecular families are of particular interest for the research objective. Therefore, in this work, the MolNetEnhacer tool was employed to track and identify the chemical classes contained in *Trichoderma spirale* (Ts) ethyl acetate extract, which has biological potential already described in the literature as bioherbicide, antioxidant, antimicrobial, antifungal, antibactericide, antitumor and larvicide using LC/Q-TOF-MS/MS and the GNPS platform (http://gnps.ucsd.edu). There were identified 111 compounds of 14 chemical classes in the network using MolNetEnhancer, where molecular families are mainly described as azoles, benzene and derivatives, carboxylic acids and derivatives, cinnamic acids and derivatives, diazines, fatty acids, flavonoids, oxanes, pirans, phenolic ethers, prenol lipids, pyrimidine nucleosides, organooxygen compounds, steroids and derivatives.

Extraction of bergenin from Peltophorum dubium extract by molecularly imprinted polymer (MIP).

https://proceedings.science/p/119704

Oscar Caetano da Silva Neto [1]
[1] UFBA

Bergenin is a gallic acid C-glycoside derivative that presents in vitro and in vivo different pharmacological and biological activities such as, anti-inflammatory, antiasthma, hepatoprotective, among others. This compound can be found in different plant families, but it is common especially in Fabaceae. Peltophorum dubium (Spreng.) Taubert (Fabaceae) is a tree popularly known as “canisfítola”, “faveira”, “angico amarela” or “farinha-seca” and its root is a source of bergenin. This work describes the preparation of a molecularly imprinted polymer (MIP) employing bergenin as an active center and submits the methanolic extract of the roots of P. dubium to isolate pure bergenin. The MIPs are synthetic material possessing specific sites and it is obtained from scaffold compounds and functional monomers that react furnishing the polymers with recognize the scaffold molecule. In the present study, the MIP was prepared employing methacrilic acid (MAA), bergenin (scaffold molecule), ethylene glycol dimethacrilate (EGDMA) as cross-linking reagent, AIBN as radical initiator and MeOH:toluene (1:1) mixture as the porogenic solvent. Sequentially, the MIP was eluted with methanol, obtaining the leached MIP. Bergenin was extracted from the methanolic extract of the roots of P. dubium, using the conventional SPE procedure employed as stationary phases the leached MIP. The leached and un-leached MIP were analyzed by IR spectroscopy and the determination of bergenin realeased was performed using HPLC/DAD analyzes with validated parameters.

Flavonoid glycosides from Fridericia speciosa Mart.

https://proceedings.science/p/120025

Juliana Cajado Souza Carvalho [1]; Inês Cordeiro [2]; Lucia Lohmann [1]; Marcelo J. P. Ferreira [3]
[1] Departamento de Botânica / Instituto de Biociências / Universidade de São Paulo; [2] Secretaria do Meio Ambiente do Estado de São Paulo; [3] USP

Few phytochemical studies were carried out from Fridericia (Bignoniaceae).
Four flavonoid glycosides were identified.
This is the first description of all compounds in the genus.

Glycosylated pyrone derivatives from fungi basidiomycete Neonothopanus gardineri and evaluation of its cytotoxic potential

https://proceedings.science/p/119946

Lhaís Caldas [1]; Mariana T. Rodrigues [1]; Ileana G.S. Rubio [1]; Cassius V. Stevani [2]; Patricia Sartorelli [3]
[1] Unifesp; [2] IQ-USP; [3] Universidade Federal de São Paulo

Neonothopanus is a bioluminescent fungi basidiomycete genus belonging to Marasmiaceae, with only two species described in the literature: N. nambi and N. gardineri. Both of them occur mainly in Australia, Malaysia and Brazil [1]. N. gardineri is known for its bioluminescence, capable of emitting green light, which metabolism is not well known up until the present [2]. In terms of the metabolites produced by this specie, only a few of them are described, being most of them terpenes, such as sesterpene, sesquiterpenes and triterpenes [3]. Therefore, this work aims to evaluate its cytotoxic potential of the methanolic extract obtained from N. gardineri against anaplastic thyroid cancer cells (KTC-2), as well as identify its metabolites. According to the results obtained, it was possible to see that the methanolic extract from N. gardineri is cytotoxic against KTC-2 at 60 µg/mL after 72 h of treatment, resulting in reduction of cell viability. O the other hand, chromatographic fractionation of methanolic extract in addition to the molecular networking and spectral library annotation generated through GNPS (Global Natural Products Social Molecular Networking), afforded the isolation of uridine (1), and the annotation of adenosine (2), nucleosides described in the literature due to its biological potential. [1] OLIVEIRA, A.G. et al. Bioluminescência de fungos: Distribuição, função e mecanismo de emissão de luz. Química Nova, 36, No. 2, 314-319, 2013. [2] CAPELARI, M. et al. Neonothopanus gardineri: A new combination for a bioluminescent agaric from Brazil. Mycologia, 103(6), 1433–1440, 2011. [3] TSARKOVA, A.S. et al. Nambiscalarane, a novel sesquiterpenoid compriding a furan ring, and other secondary metabolites from bioluminescent fungus neonothopanus nambi. Mandeleev Communications. 26, 191-192, 2016.

Green approach for optimization of bioethanol-based HPLC-PAD method for E. uniflora metabolomic fingerprint and biomimetic microwave-assisted-extraction in natural deep eutectic solvents (NADES)

https://proceedings.science/p/120321

Otávio Aguiar de Souza [1]
[1] Universidade Estadual Paulista 'Julio de Mesquita Filho'

Identificação de flavonóides por CLAE e avaliação da atividade citotóxica de folhas e flores de P. neochilus Schltr.

https://proceedings.science/p/120384

Mariana das Graças Augusta César [1]; Alexandre Milanez Brandão [1]; Roqueline Rodrigues Silva [1]; Cecilia de Souza O. Bento [2]; Patrícia Oliveira Machado [1]; Adriano P. Sabino [2]; Fernanda C. G. Evangelista [2]

[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Universidade Federal de Minas Gerais

Identification of flavonoids by HPLC and evaluation of the cytotoxic activity of leaves and flowers of P. neochilus. Report of flavonoids from extracts of flowers and leaves of Plectranthus neochilus.

Identificação química e avaliação antitumoral do extrato hidroalcoólico de Coriandrum Sativum contra a linha celular SH-SY5Y.

https://proceedings.science/p/120724

Milena Fernandes Santos [1]; Daniel Moreno Garcia [2]; Daniel Spindola [2]; Leila Yumi Kato de Santana [2]; Victor Cavalaro [2]; Vitor Binda [2]; Ana C. de Carvalho [3]; THIAGO VEIGA [4]; Livia Soman de Medeiros [4]; Lucas Zamarioli [2]; Maria Cristina Marcucci [5]; Carlos Rocha Oliveira [2]; Simone dos S. Grecco [1]

[1] Universidade Anhanguera de São Paulo; [2] Universidade Anhembi Morumbi; [3] UNIFESP; [4] Universidade Federal de São Paulo; [5] Universidade Estadual Paulista - UNESP

Coriandrum sativum L. (Apiaceae), popularly known as coriander (“coentro” in Brazil) and for presenting a strongly aromatic fragrancy, and exotic slightly sweet flavor, favoring it use as a condiment in the cuisine of different parts of the world. Its aromatic, nutritional and therapeutic properties are due to the chemical composition of its different plant parts1. However, the most studied part and, therefore, with greater indications are its fruits/seeds. Studies highlight the antimicrobial, antioxidant, hypoglycemic, hypolipidemic, anxiolytic, analgesic, anti-inflammatory, anticonvulsant and anticancer potential of coriander2. Although there are reports about its antitumor activity3, especially of its seeds, against breast and prostate cancer cells, so far, no study has evaluated the antitumor potential of its leaves against the human neuroblastoma lineage. Thus, herein the hydroethanolic extract from all parts of coriander (CSHE) were subjected to UPLC/DAD-ESI/HRMS/MS analysis and evaluation of its cytotoxicity and cell death mechanism against neuroblastoma cell line of bone marrow (SH-SY5Y). The IC50 value of CSHE against SH-SY5Y cell line was defined as 20 mg/mL. In addition, the annexin V/propidium iodide assay suggested apoptosis as cell death mechanism. Those results can be explained by the chemical investigation, especially for isocoumarins (coriandrin, dihydrocoriandrin and coriandrone) purines (adenin and adenosine), aminoacid (tryptophan), flavonoids (rutin and apigenin), phospholipids (PAF C-16 and LysoPC - 16:0) and acylglicerol (monolinolenin) found at this extract. In conclusion, further experiments are necessary to determine whether those bioactive compounds act in synergism or an isolated compound could be the main responsible for the antitumoral activity.

Identification and synthesis of bombykol and its derivative acetate as the aggregation pheromone of Montella sp. (COLEOPTERA: CURCULINIDAE)

https://proceedings.science/p/119972

Rândilla Regis Cordeiro dos Santos [1]; Jessica Jordão [2]; Carla Fernanda Favaro [2]; Paulo Zarbin [1]

[1] Universidade Federal do Paraná; [2] Universidade Estadual de Santa Cruz

The extracts from males of Montella sp. have three male specific compounds, bombykol and its derivative bombykyl acetate (EZ and EE). The synthetics compounds were bioactive in the bioassays tests.

Identification of bisresorcinol derivatives in wood residues from Roupala montana (Aubl) and activity against Cryptococcus

https://proceedings.science/p/119830

Maria da Paz Lima [1]

[1] Instituto Nacional de pesquisas da Amazônia

The chromatographic fractionation of the methanolic extract from wood residues of Roupala montana led to the isolation of bisresocinol derivatives with activity against the fungi Cryptococcus neoforma

Identification of compounds present in two different Caatinga medicinal plants obtained in free markets in Senhor do Bonfim x0096 BA

https://proceedings.science/p/120252

Vitor Silva Melo; Ezequiel Ribeiro dos Santos [1]; Gabriel Luiz da Silva [2]; Fabiano Reis Amorim Júnior [1]; José Carlos Bispo da Silva Filho [1]; Pérsio Alexandre da Silva [3]; Cláudia Sampaio de Andrade Lima [3]; Liliane Gallindo Dantas [1]; Gustavo Frenshc [1]

[1] UNIVASF; [2] Universidade Federal do Vale do São Francisco; [3] UFPE

Identification of compounds present in two different Caatinga medicinal plants obtained in free markets in Senhor do Bonfim – BA Highlights We identified compounds present in several samples of two medicinal plants. Compounds had a high variation between samples, which can mean adulteration, misidentification or storage error. Resumo/Abstract Medicinal plants of Brazilian native flora are consumed with little or no proof of its pharmacological properties, based only on users' or traders' reports. Although they are natural and, therefore, popularly considered free of side effects, medicinal plants' toxicity is a serious public health concern, either because of the plant's own compounds, either by adulterations or interaction with other medicines.1 Since these medicinal plants are usually sold in markets and free fairs by people without formal education, there may be labeling or manipulation problems, resulting in the absence of the desired effects or presence of adverse effects.1 These plants should have stricter control regarding the plant origin, time since it was harvested, way of collection, storage, drying and packing, and contamination presence. 2 In this work we identified compounds present in different medicinal plants samples found in Senhor do Bonfim free market (BA): six samples of Sene (Senna alexandrina; Fabaceae) and six samples of Umburana (Commiphora leptophloeo; Burseraceae). For the extraction of the compounds in sene, we used hydrodestilation, and for umburana we extracted the compounds using maceration with hexane. All extracts were analyzed by GC-MS. The main compounds present in sene extracts were n-hexadecanoic acid (49,79-84,64%), (Z,Z,Z)-9,12,15- octadecatrienoic acid (1,97-13,2%), tetradecanoic acid (2,15-4,57%), and two unidentified compounds in 1,89-11,95% and 1,45-8,49%. For umburana, the compounds present were octadec-9-enoic acid (34,56- 63,14%), cumarin (5,57-48,27%), n-hexadecanoic acid (4,93-8,32%), octadecanoic acid (2,11-3,79%) and two unidentified compounds in 3,38-7,35% and 3,48-8,97%. As we can see, compounds in both plants had a high variation between samples, which can mean either that some of the medicinal plants sold in free markets belong to a species different from the announced one or, at least, that compounds found in the sample had degraded between harvest and sale. Further analysis in molecular level will define if all samples are from the same species. Genotoxicity and cytotoxicity tests will be done with all samples in the future in order to confront chemical and toxicity data. References 1. VEIGA JUNIOR, V. F.et al. Plantas Medicinais: Cura Segura? Quim. Nova, v. 28, n. 3, p. 519–528, 2005. 2. USTULIN, M. et al. Plantas medicinais comercializadas no Mercado Municipal de Campo Grande-MS Revista Brasileira de Farmacognosia, scielo, 2009. Agradecimentos/Acknowledgments The authors thank CNPq and FAPESB for financial support and scholarships. We also thank ITCBio for the GC-MS analysis.

Identification of the sex and alarm pheromones of the sheldbugs, Orsilochides leucoptera (HEMIPTERA: SCUTELLERIDAE)

https://proceedings.science/p/120396

Douglas José de Melo [1]; Maycon Silva [1]; Antonioni Moliterno [1]; Paulo Zarbin [1]

[1] Universidade Federal do Paraná

The amazing ability of stinkbug to release high amounts of strong-smelling and irritating defensive compounds is related to its metathoracic gland, which is an exocrine gland with defensive, sexual, alarm and aggregation signals function. Orsilochides leucoptera (Scutelleridae) is widespread species in the Neotropical region, which has been found as host in plants of the families as Malvaceae, Poaceae and Euphorbiaceae. Inside the large family of true bugs Scutelleridae, metathoracic gland secretion have been investigated for three species and a series of compounds as ketones, acetone, alcohols and esters were identified. However, no sex pheromone compound have been described for any species of Scutelleridae, Therefore, the aim of this work was to give the first steps in the studies of sex pheromone communication within this large family of stink bugs, as well as to identified the compounds present in the MTG of O. leucoptera. GC/MS analysis revealed two male sex specific compounds identified as (R)-camphor and (R)-borneol, which showed high attractivity to females in Y-tube olfactometer bioassays. Also, based on GC/MS analysis of secretions from MTG of males and females of O. leucoptera, additionals eight compounds were identified: 2-(E)-hexenal, (E)-4-oxo-2-hexenal, (E)-hex-2-enyl acetate, (R)-linalool, (R)-α-terpineol, dodecane, 1-tridecene and n-tridecane. From these, compound (R)-α-terpineol has been detected only in the glands of males. Most of the methatoracic gland compounds identified in O. leucoptera have been usually identified in Heteroptera species. Camphor is related to be toxic and repellent for insects, even though, here for the first time, this compound is identified as a sex pheromone in insects.

Identification of volatiles produced by Nasutitermes corniger (Isoptera: Termitidae) soldiers

https://proceedings.science/p/119835

Gustavo Frensch [1]; Gabriel Luiz da Silva [1]; Fabiano Reis Amorim Júnior [1]; José Carlos Bispo da Silva Filho [1]; Vitor Silva Melo [1]; Ezequiel Ribeiro dos Santos [1]; Pérsio Alexandre da Silva [2]; Liliane Gallindo Dantas [1]; Virgínia Farias Pereira de Araújo [1]; Cláudia Sampaio de Andrade Lima [2]

[1] Universidade Federal do Vale do São Francisco; [2] Universidade Federal de Pernambuco

Highlights In this work, we discovered that Nasutitermes corniger soldiers, when isolated, produced Methyl Salicilate, whereas when aerated with an individual from another colony, produced a great amount of Eugenol. Abstract Chemicals involved in communication between organisms are called infochemicals, which can be classified as intraspecific (phemoromes) or interspecific (alelochemicals).1 For eusocial insects, such as termites, pheromones are involved in every aspect of live, as reproduction, foraging, defense, orientation, and every other interaction in the colony.2 Termites, for example, produce alarm, sexual, trail and aggregation, among others pheromone classes.3 In this work, we identified volatile compounds produced by soldiers of N. corniger from four different nests in a 100 m2 area in the city of Campo Formoso-BA. Prior to volatiles extraction, we performed behavioral tests. Ten soldiers of each nest were placed in a petri dish and then ten soldiers of another nest were placed in the same petri dish. All nest combinations were tested, and, in every experiment, termites showed aggressive behavior. For volatiles extraction there were two different treatments: 1) around 100 isolated soldiers from each nest and 2) about 100 soldiers of one nest with 5 soldiers of a different colony. Individuals were placed in aeration chambers for 24h and the volatiles were trapped on a 0.4 cm long bed of Super Q resin (Allthec, Deerfield, Illinois USA), which was latter eluted with hexane. Extracts were concentrated as required under Ar and were analyzed by GC-MS. On the first treatment, all colonies' soldiers produced mainly Methyl Salicilate. For the second treatment, Methyl Salicilate was still produced but there was also production of Eugenol in a greater amount (87%). Although behavior tests are still up to be done, we can infer that Methyl Salicilate may be an aggregation pheromone and Eugenol may be an alarm pheromone or a defensive compound. Those behavior tests may determine the real function of each compound. References

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In vitro assessment of drug metabolism and pharmacokinetic (DMPK) properties in drug discovery: examples of marine and plant natural products

https://proceedings.science/p/119691

Rodrigo Moreira Silva [1]; Daniel B. Carrão [1]; Simone S. Fortes [1]; Anderson R. M. de Oliveria [1]; Denise Brentan Silva [2]; Alberto J. Cavalheiro [3]; Paula C. Jimenez [4]; William Fenical [5]; Letícia V. Costa-Lotufo [1]; Norberto P. Lopes [1]

[1] USP; [2] UFMS; [3] UNESP; [4] UNIFESP; [5] UCSD

In addition to adequate pharmacological efficacy and safety profile, a balance of optimized bioavailability and reduced drug interactions potential maximizes the chance of a natural product becoming a successful therapy. Drug metabolism and pharmacokinetic (DMPK) screening must be evaluated firstly in vitro, which provides pharmacological orientation for in vivo design studies. Considering the demand for innovative products from Brazilian biodiversity, a platform for preclinical studies of natural products was developed by our research group, in which in vitro DMPK assays were applied to lead compounds with highlighted in vitro pharmacological activity such as seriniquinone (marine natural product), specioside, casearin X and licarin A (plant natural products). The compounds were evaluated for determination of its lipophilicity (shake-flask method), permeability (Caco-2 cells monolayer system), plasma protein binding (ultracentrifugation), metabolites survey (Human Liver Microsomes – HLM; metalloporphyrins; Electrochemistry-Mass Spectrometry) and kinetic parameters of metabolism, phenotyping and drug interactions studies (HLM) - Table 1. Table 1 – In vitro DMPK main results obtained for seriniquinone, specioside, casearin X and licarin A. Compound seriniquinone specioside casearin X licarin A Structural class Quinone Iridoid glycoside Clerodane diterpene neolignan Log P 4.5 -1.6 5.9 3.8 Apparent permeability (x10-6cm/s) 3.9 (moderate) 11.2 (high) 0.0 / 66.9* - Plasma protein binding (%) 80.1 43.3 87.3 26.0 Hepatic clearance (mL/min/kg) 6.1 (moderate) 2.4 (low) 19.5 (high) 20.0 (high) Metabolic stability: half-life (min.) 40.2 59.7 8.7 31.5 Metabolism phenotyping CYP1A2, 2E1

CYP1A2 carboxylesterase CYP1A2, 2B6 Number of metabolites elucidated 0 1 1 7 Drug interactions Isoforms inhibited CYP1A2, 2E1, 3A CYP1A2 Not applicable CYP1A2 IC50 (µmol/L) < 1.5 (strong) 100.0 (weak) Not applicable 87.0 (weak) Recommendations for next steps In vivo PK In vivo PK Chemical modification Formulation development *Performed in intact Caco-2 cells system / Caco-2 cells with carboxylesterases inhibited. This platform provides a data panel that allows identifying key areas in which properties of compounds needs to be improved or to proceed through in vivo PK. Thereby, in vitro DMPK screening for potential compound classes allows the researcher team to rank order of molecules not only based on their potency, but also in relation to the predicted bioavailability, which is crucial for the advance on drug discovery and development from natural sources.

In vitro evaluation of the antitrypanosomal activity of diterpenes and sesquiterpenes isolated from Baccharis sphenophylla (Asteraceae)

https://proceedings.science/p/119743

Joao Lago [1]; Matheus Lopes Silva [1]; Juliana Brito [2]; Guilherme Antar [3]; Thais Costa-Silva [1]; André Gustavo Tempone [4]
[1] Universidade Federal do ABC; [2] Instituto de Ciências Ambientais, Químicas e Farmacêuticas / Universidade Federal de São Paulo; [3] Universidade de São Paulo; [4] Adolfo Lutz

The phytochemical study from Baccharis sphenophylla afforded four diterpenes (1 – 4) and two sesquiterpenes (5 – 6). Compounds 2 – 5 displayed activity against trypomastigote forms of T. cruzi.

Insecticidal activity of essential oils of Pelargonium graveolens l'Herit and Lippia alba (Mill) N. E. Brown against Spodoptera frugiperda (J. E. Smith)

https://proceedings.science/p/120066

Edenilson dos Santos Niculau [1]; Péricles Barreto Alves [1]; Paulo Nogueira [2]; Valéria Regina de Moraes [1]; Andreia Matos [3]; João Batista Fernandes [3]; Maria Fátima das Graças Fernandes da Silva [3]; Arlene Gonçalves Corrêa [3]; Arie Blank [1]; Leandro do Prado Ribeiro [4]
[1] Universidade Federal do Tocantins; [2] Universidade Federal de Sergipe; [3] Universidade Federal de São Carlos; [4] Empresa de Pesquisa Agropecuária e Extensão Rural de Santa Catarina/Centro de Pesquisa para Agricultura Familiar
Lippia alba (Mill) N. E. Brown and *Pelargonium graveolens* L'Herit are major producers of essential oils (E.O) and have several applications, mainly in the perfumery, cosmetics and pharmaceutical industries. *L. alba* is an aromatic medicinal plant that occurs in almost all regions of Brazil. Several volatile compounds are present in the E. O of this plant, among which stand out: citral (geranial + neral), linalool, limonene, carvone, camphor and 1,8-cineole. *P. graveolens* is known as fragrant mallow or geranium and was introduced in India in the early 20th century. Citronellol, geraniol, linalool and citronellate formate are the main components present in oil essential of this species. In this work, insecticidal activity of E. O of *Pelargonium graveolens*, *Lippia alba* and compounds geraniol, linalool, 1,8-cineole, limonene, carvone, citral and Azamax® were evaluated against *Spodoptera frugiperda*. Topical application assay showed E. O of *P. graveolens* has acute toxicity against *Spodoptera frugiperda* larvae (third instar) with LD50 1.13 µg/mg per insect and LD90 2.56 µg/mg per insect. Three E. O of *L. alba* also exhibited insecticidal activity with LD50 ranging from 1.20 to 1.56 µg/mg per insect and LD90 from 2.60 to 3.75 µg/mg per insect (Table 1).Geraniol, linalool, carvone and citral caused significant mortality of 30, 90, 84 and 64% respectively, compared to negative control. The bioinsecticide, Azamax®, caused lower mortality than the compounds of the E. O.

Integrated analytical approaches for accessing bioactive compounds from Swinglea glutinosa (RUTACEAE) and its associated fungi

https://proceedings.science/p/120656

THIAGO VEIGA [1]; Ana Carvalho [1]; Claudio Yoshio Ogawa Junior [1]; Lívia Soman de Medeiros [1]
[1] Universidade Federal de São Paulo
Nesta conferência serão apresentados os resultados referentes ao estudo químico da espécie *Swinglea glutinosa*, uma planta da família Rutaceae. As abordagens de desreplicação via HRMS permitiu o isolamente de acridonas e fenilacrilamidas com potencial anti-leucemia. Além disso, o microbioma da espécie está sendo explorado através do isolamento de seus fungos endofíticos. Uma nova espécie de *Penicillium* foi obtida e por meio da plataforma GNPS, foram identificados putativamente metabólitos clorados, possivelmente pertencentes à classe das antraquinonas.

Integrated Analytical Tools for Discovering Anti-Leukemia Metabolites from Urena lobata L. (Malvaceae)

https://proceedings.science/p/119821

Fernando Cassas [1]; Fernando Cassas [1]; Heron V. Torquato [2]; Wagner D. S. Vital [2]; Edgar J. Paredes-Gamero [3]; Livia Soman de Medeiros [4]; THIAGO VEIGA [4]

[1] Universidade Federal de São Paulo; [2] Department of Biochemistry, Federal University of São Paulo – UNIFESP; [3] Faculty of Pharmaceutical Sciences, Food and Nutrition - Federal University of Mato Grosso do Sul – UFMS, Brazil; [4] Otto Richard Gottlieb Bioorganic Chemistry Lab, Department of Chemistry, Federal University of São Paulo - UNIFESP

Crude extracts obtained from Urena lobata L. were submitted to anti-leukemia assays. Among them, dichloromethane extract from the aerial parts was selected to start our chemical approach. Based on this, the study is being performed using two rapid dereplication strategies: Target Analysis (Bruker Daltonics®) MS data analysis combined with MS/MS data obtained from GNPS platform. Preliminary data showed the presence of different classes of Natural Products in the cytotoxic extracts. The combination of hyphenated techniques may increase the efficiency and speed of analysis, being useful tools to access unrevealed natural products (NPs), which include molecular dereplication 1,2. In this sense, our goal is the employing of integrated analytical techniques to accelerate the discovery of metabolites (unknown or not) from Urena lobata L., guided by anti-leukemia assays. For this, different human leukemia cells were employed in an initial screening: Raji (Lymphocyte B), CCRF-CEM (Acute Lymphoblastic Leukemia) and Kasumi-1 (Acute Myeloid Leukemia). The cytotoxic assays (during 24 hours at 100 µg/mL) allowed us to select the dichloromethane extract from the aerial parts of U. lobata L. (ULD). After a chromatographic column (on silica flash), ten subfractions from ULD (2,0 g) were obtained; all of them were submitted to the cytotoxic evaluation again. Most of them practically inhibited at least 85% of the leukemia cells proliferation. Our UHPLC-MS analyzes revealed the presence of more than 100 ions present in the subfractions. Through the integrated tools we were able to find some compounds related and also unrelated in the literature for the species, for example, urenalobaside A, glycosilated urenoside and hydroquinidine which reveals, therefore, good perspectives for discovering anti-leukemia and/or unrelated NPs from U. lobata L. 1 Carvalho, A.; Rodrigues, L.; Ribeiro, A.; Silva, M.; Medeiros, L.; Veiga, T. Integrated Analytical Tools for Accessing Acridones and Unrelated Phenylacrylamides from Swinglea glutinosa. Molecules 2020, 25, 153 2 Van Herwerden, Eric F.; Süssmuth, Roderich D. Sources for Leads: Natural products and libraries. In: New Approaches to Drug Discovery. Springer International Publishing, 2015. p. 91-123.

Intraspecific evaluation of the chemical composition and antibacterial activity of essential oils from the leaves of Croton argyrophyllus (Euphorbiaceae).

https://proceedings.science/p/120199

LIDIANE GOMES DE ARAÚJO [1]; Maria da Conceição de Menezes Torres [2]; J. V. O., Alves [3]; Bruno Oliveira de Veras [4]; Márcia Vanusa da Silva [4]; José Filipe Bacalhau Rodrigues [5]; Solomon Kweku Sagoe Amoah [5]; Gleyton Leonel Silva Sousa [6]

[1] Universidade Estadual da Paraíba - UEPB; [2] UEPB; [3] Departamento de bioquímica / Laboratório de Produtos Naturais / Universidade Federal de Pernambuco; [4] Universidade Federal de Pernambuco - UFPE; [5] Universidade Federal de Campina Grande; [6] Programa de Pós-Graduação em Química / INSTITUTO DE QUÍMICA / Universidade Federal Rural do Rio de Janeiro

Extraction of essential oil from nine samples of Croton argyrophyllus by hydrodistillation. Intraspecific evaluation of the chemical composition by CG / MS and antibacterial activity against Staphloco

Investigation of metabolic profile of common bean (P. vulgaris) treated with a biofertilizer obtained through fermentation of Corynebacterium glutamicum

https://proceedings.science/p/120715

Stephanie Nemesio da Silva [1]; Taicia Pacheco Fill [1]; Rodrigo Alberto Repke [2]; Rafael Leiria Nunes [2]

[1] Universidade Estadual de Campinas; [2] Outros

This study evaluated the metabolic profile of leaf extract of Phaseolus vulgaris treated with a biofertilizer obtained from Corynebacterium glutamicum using the molecular networking tool.

Ishwarane, ishwarone and ishwarol: rare sesquiterpenes in Piper alatipetiolatum essential oil
https://proceedings.science/p/120719

André Correa de Oliveira; Rosemary Aparecida Roque [1]; Sergio Massayoshi Nunomura [1]; Rita C. Saraiva Nunomura [2]
[1] Instituto Nacional de Pesquisas da Amazônia; [2] Universidade Federal do Amazonas

Ishwarane, ishwarol-B, and ishwarone were identified in the essential oil of Piper alatipetiolatum by GC-FID, GC-MS, and 13C NMR. The essential oil also inhibited the enzyme acetylcholinesterase.

Isolamento bioguiado de substâncias com potencial atividade antimicrobiana de extratos etanólicos de Geoprópolis produzida por Melipona rufiventris
https://proceedings.science/p/120733

Rafael Ferreira [1]; Lidiane Lázaro [1]; Lucas Pires [1]; Rosane Nora [1]
[1] Universidade Federal Rural do Rio de Janeiro

The main objective of this work was to identify and isolate substances with potential antimicrobial activity of geopropolis of stingless bees of the species melipona rufiventris (uruçu-amarela).

Isolation and identification of secondary metabolites produced by the endophytic fungus Epicoccum sp associated with Disynaphia filifolia
https://proceedings.science/p/119720

Nathália Malaco [1]; Anderson Valdiney Gomes Ramos [1]; Andressa Domingos Polli [1]; Adriano Borges Meniqueti [1]; Thomas Kehrwald Fruet [1]; Maria Helena Sarrragiotto [1]; João Alencar Pamphile [1]; Debora Cristina Baldoqui [1]
[1] Universidade Estadual de Maringá

First isolation of endophytic fungi from Disynaphia filifolia. Four compounds identified from Epicoccum sp. First detection of the yellow pigment macrosporin in Epicoccum.

Isoprenoides da fração hexânica das folhas de Machaerium acutifolium Vogel
https://proceedings.science/p/120205

Jurema Santana de Freitas [1]; Adonias Almeida Carvalho [1]; Lucivania Rodrigues dos Santos [1]; Rodrigo Ferreira Santiago [1]; Bruno Quirino Araújo [2]; Mariana Helena Chaves [1]
[1] Universidade Federal do Piauí; [2] Universidade Federal do Espírito Santo

Machaerium acutifolium (Fabaceae-Papilionoideae) é conhecida popularmente por jacarandá do campo, jacarandá-caroba e jacarandá bico-de-pato. No Brasil, ocorre da Amazônia até São Paulo e também no Mato Grosso do Sul, Bahia, Piauí e Maranhão, principalmente na área de cerrado. Esta espécie é tradicionalmente usada como contraceptivo, para tratar menstruação dolorosa e dores estomacais. O tronco de M. acutifolium contém polifenois (éter monometílico de pinosilvina, (+)-medicarpina e petroestireno). Em estudos anteriores com as folhas foram identificados flavonoides: canferol-3-O-rutinosil-7-O-diraminosídeo, quercetina-3-O-rutinosil-7-O-ramnosídeo, rutina, canferol-3-O-rutinosídeo, canferol-3-O-glicosídeo e isoflavonoides: daidzeína-8-C-glicosídeo e genisteína. A fração hexânica (FHFMa) foi obtida da partição do extrato etanólico das folhas de M. acutifolium. Uma alíquota de FHFMa (10 g) foi submetida a processos cromatográficos sucessivos, possibilitando o isolamento e/ou identificação de 7 triterpenoides: 3-O-(E)-cumaroil-β-amirina (1), 3-O-(Z)-cumaroil-β-amirina (2), 3-O-(E)-cumaroilgermanicol (3), 3-O-(Z)-cumaroilgermanicol (4), 3-O-(E)-cumaroil-lupeol (5), 3-O-(Z)-cumaroil-lupeol (6) e lupeol (7), 4 esteroides: colesterol (8), campesterol (9), sitosterol (10), estigmasterol (11) e um tocoferol: α-tocoferol (12). Os compostos 7-11 foram identificados por CG-EM, a partir dos derivados sililados. Os compostos foram identificados com base em dados de Ressonância Magnética Nuclear de hidrogênio, carbono-13 e DEPTQ e por comparação com dados da literatura. Este é o primeiro relato dos compostos (1-6, 8, 9, 11 e 12) no gênero Machaerium.

Isoprenoides da fração hexânica das folhas de Senna acuruensis Benth

https://proceedings.science/p/120206

Rodrigo Ferreira Santiago [1]; Lucivania Rodrigues dos Santos [2]; Jurema Santana de Freitas [1]; Luanda Ferreira Floro da Silva [2]; Adonias Almeida Carvalho [1]; Mariana Helena Chaves [2]

[1] Universidade Federal do Piauí; [2] Universidade Federal do Piauí - UFPI

Senna acuruensis Benth (sin. Cassia acuruensis), pertencente à família Fabaceae, subfamília Caesalpinoideae, é conhecida popularmente como canela de velho ou besouro. É uma espécie nativa e endêmica do Brasil, distribuída nos estados da Bahia, Alagoas, Pernambuco, Sergipe e Piauí. Em estudos anteriores os extratos etanólico e aquoso desta espécie apresentaram atividade antioxidante frente aos radicais DPPH, óxido nítrico, hidroxila e peroxila, enquanto os extratos hexânico e etanólico apresentaram atividade anticolinesterásica. Adicionalmente, os flavonoides rutina e quercetina foram quantificados por cromatografia líquida de alta eficiência nos extratos etanólico, aquoso e fração hidrometanólica das folhas.4 Como parte das investigações sobre metabólitos secundários de espécies do cerrado piauiense, este trabalho teve como objetivo realizar o isolamento e identificação estrutural de constituintes químicos do extrato etanólico das folhas de *S. acuruensis*. As folhas da espécie foram coletadas em Jatobá do Piauí-PI e uma exsicata foi depositada no Herbário Graziela Barroso-UFPI, com o número TEPB 17193. As folhas moídas (801 g) foram submetida à maceração com etanol fornecendo o extrato etanólico (EESa, 46,5 g). Uma alíquota de 30 g foi suspensa em MeOH/H2O (1:2) e extraída com hexano, obtendo-se as frações hexânica (FHSa, 20 g) e hidrometanólica (FHMSa, 9,2 g). A FHSa (10 g) foi submetida a processos cromatográficos sucessivos levando ao isolamento do diterpeno: 3,7,11,16-tetrametil-hexadecan-1,2-diol (**1**), dos triterpenoides: esqualeno (**2**), lupeol (**3**), α-amirina (4), β-amirina (**5**), germanicol (**6**), ácido canárico (**7**), ácido 3,4-*seco*germanican-3-oico (**8**) e ácido nictântico (**9**), dos esteroides: sitosterol (**10**) e estigmasterol (**11**) (Figura 1). A identificação estrutural dos compostos foi feita com base em dados espectroscópicos de Ressonância Magnética Nuclear de hidrogênio e carbono-13, uni e bidimensionais e em comparação com dados da literatura. Este é o primeiro relato destes compostos na espécie S. acuruensis, de **1** e **6**-**9** no gênero *Senna*.

Isoquinoline Alkaloids from the Leaves of Duguetia pycnastera (Annonaceae)

https://proceedings.science/p/119675

Victória Brandão Nardelli [1]; César Augusto Silva de Souza [1]; Felipe Moura Araújo da Silva [2]; Hector Henrique Ferreira Koolen [3]; Emmanoel Costa [1]

[1] Departamento de Química, DQ/UFAM, Manaus-AM; [2] Central Analítica, CA/UFAM, Manaus-AM; [3] Escola Superior de Ciências da Saúde

1. Isoquinoline alkaloids were found in the leaves of Duguetia pycnastera (Annonacea); 2. The alkaloids belong to the aporphine, oxoaporphine and tetrahydroprotoberberine alkaloids types; 3. The identified alkaloids are described for the first time in the leaves of this species; 4. The obtained results reinforce the chemosystematics proposed for the Annonaceae family.

Labdane diterpenes from the aerial parts of Lomatozona artemisiifolia Baker

https://proceedings.science/p/119964

Vinícius Galvão Wakui [1]; Lorrant Marcos Abreu [1]; Ana Paula Terezan [1]; Cecília Maria Alves de Oliveira [1]; Sérgio Tadeu Sibov [1]; Lucilia Kato [1]

[1] Universidade Federal de Goiás

Lomatozona artemisiifolia Baker (Asteraceae) is an endemic specie from the Cerrado of Goiás state. It has been included in the red list of Brazilian flora threatened with extinction1, and concerning its conservation in the Cerrado biome, it was realized a study of cultivation and in vitro micropropagation. Recently its AcOEt extract had been evaluated against the nematodes Pratylenchus bachyurus and Melodoigyne javanica2, which have caused serious damage to cultures of tomatoes and soy, showing promising results. In this work we have identified of a series of labdane diterpenes in the extracts of L. artemisiifolia. The aerial parts were submitted to an extraction following the procedures described in a previous work3, affording three extracts: ethyl acetate 1 (EA1), ethyl acetate 2 (EA2) and ethanolic (EE), from vegetal material collected in a dry and wet season, and also for the in vitro micropropagated plant. Additionally, it was prepared the hexane extract (HE) from the EA1, using n-hexane. The EA1 extract from dry season was submitted to successive chromatographic columns, using silica gel 60 and a mixture of CHCl3/MeOH (100:0 to 50:50), affording compounds 1 and 2. The same procedure was adopted for HE extract, leading to the isolation of compounds 1 and 3. These compounds showed positive reaction the diterpene class in the TLC analysis and were characterized through 1D and 2D NMR techniques. The HMBC experiment confirmed the decaline system by long

range correlations of the methyl groups at dH 0.86 (s) (H-18) and dH 0.79 (s) (H-19) with the carbons C-3 (dH 1.37/1.14 (m); dC 33.5) and C-5 (dH 0.91 (m); dC 56.3), as well as the methyl group at dH 079 (s) (H-20) with carbons at C-1 (dH 1.60/0.93; dC 39.7), C-5 (dH 0.91 (m); dC 56.3) and C-9 (dH 1.00 (t, 3.7 Hz); dC 62.3). Compounds 1 and 2 also showed multiplets at dH 3.6 (H-15) and dH 4.1 (H-15), respectively, while compound 3 signals of two doublets of doublets at dH 2.33 (14.7 and 6.1 Hz, H-14) and dH 2.19 (14.7 and 7.6 Hz, H-14), indicating the presence of a side chain in these diterpenes, characterized by the correlation of dH 1,00 (t, 3.7 Hz) with the carbon at dC 40.9 (C-12). These compounds were identified as 8,15-labdanediol (1), its acetyl derivative (2) and labdanolic acid (3), by comparison with literature4,5, reported for the first time in this specie and genus. Furthermore all extracts were analyzed through LC-MS/MS and data from EA1 and EE extracts were submitted to a molecular networking analysis using GNPS platform, leading to the annotation of 8,15-labdanediol (1) and 8-hydroxylabdan-15-oic acid (3) in the in vitro EA1 and dry season EE extracts, respectively. The perspectives of this work is the evaluation of the nematicide activity of all extracts from L. artemisiifolia, and the correlation of these results with the identified compounds through a chemometric analysis. References: 1. Nakajima, J. N. et al. Rodriguésia 2012, 63, 39-54; 2. Silva, L. C. da. PhD thesis, UFG, 2019; 3. Kato, L. et al. 41a RASBQ 2018; 4. Gárcia-Sanchéz, E. et al. Journal of Natural Products 2014, 77, 1005-1012; 5. Mahadeo, K. Journal of Natural Products 2019, 82, 1361-1366.

Metabolic profile analysis of Fabaceae plant species from Caatinga biome using metabolomic tools

https://proceedings.science/p/119661

Danielle Rocha Pinho Barros [1]; Alan Cesar Pilon [2]; Tomas Ferreira Domingues [3]; Jonathan Lloyd [4]; Norberto Peporine Lopes [3]

[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP); [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Universidade de São Paulo; [4] Imperial College London

Chemical Mapping of species belonging to Fabaceae in the Caatinga.
Use of GNPS and ChemRICH in the search for metabolic patterns.

Microwave and ultrasound extraction of antioxidant compounds from Croton grewioides: optimization using response surface method.

https://proceedings.science/p/119412

Valéria Regina de Moraes [1]; Pedro Ellison Santos do Nascimento [1]; Raphael Amancio de Jesus [1]; José Carlos Freitas de Sá Filho [1]; Sara Dayan da Silva Oliveira [1]; Cristivane Lima [1]; Arie Blank [1]; Paulo Nogueira [1]; Vilma Prado [1]

[1] Universidade Federal de Sergipe

Optimization of the extraction processes of the phenolic compounds of the species C. grewioides, using ultrasound and microwaves to determine the antioxidant capacity of the species.

Molecular dereplication and anti-Trypanosoma cruzi activity evaluation of essential oils from different parts of Saururus cernuus L. (Saururaceae)

https://proceedings.science/p/119558

Juliana Brito [1]; João Henrique Ghilardi Lago [2]; Edgard Antonio Ferreira [3]; Thais Costa-Silva [4]; André Gustavo Tempone [5]; Patricia Sartorelli [6]; Leticia Ferreira Lima [7]

[1] Instituto de Ciências Ambientais, Químicas e Farmacêuticas / Universidade Federal de São Paulo; [2] Universidade Federal do ABC; [3] Escola de Engenharia / Universidade Presbiteriana Mackenzie; [4] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC; [5] Adolfo Lutz; [6] Universidade Federal de São Paulo; [7] Universidade Presbiteriana Mackenzie

In this work, the molecular dereplication of essential oils from inflorescences, leaves, branches and roots of Saururus cernuus was performed and the anti-Trypanosoma cruzi activity was evaluated.

Molecular dereplication and cytotoxic effects of extracts from leaves of Nectandra barbellata (Lauraceae) and related costic/isocostic acids

https://proceedings.science/p/120034

Kaio Gomes [1]; Vinicius Silva Londero [2]; Giselle Cerchiaro [1]; Carlos Rogério de Figueiredo [2]; João Henrique Ghilardi Lago [3]

[1] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC; [2] Universidade Federal de São Paulo; [3] Universidade Federal do ABC

Molecular dereplication of cytotoxic extracts from leaves of N. barbellata was performed by NMR and indicated the predominance of costic/isocostic acids. These compounds exhibited antitumor activity

Novel Cytotoxic Chromenones from Kielmeyera reticulata (Calophyllaceae)

https://proceedings.science/p/120272

Milena Oliveira [1]; Florisvaldo Ramos [1]; Elisangela Boffo [1]; Ramón El-Bachá [1]; Frederico Guaré [1]; Heiter Valverde Magalhães Boness [1]

[1] Universidade Federal da Bahia

The genus *Kielmeyera* (Calophyllaceae) aggregates 47 Brazilian native species that are found in the biomes of Cerrado, Restinga, and Campo Rupestre. Previous studies with *Kielmeyera* species have revealed the occurrence mainly of xanthones, 4-phenyl, and 4-alkylcoumarins. In this work, we describe the isolation and structural determination of novel 4-alkylchromenones from *K. reticulata* as well as we have evaluated their cytotoxic activity against rat glioma (C6) cell line.

Novo alcaloide anti-inflamatório isolado de Ocotea diospyrifolia (Meins.) Mez

https://proceedings.science/p/120721

Nátalie de Barros Vieira [1]; Aline de Fátima Silva [1]; Karen de Jesus Nicácio [1]; Danielle Ferreira Dias [1]; Marisi Soares [1]; Daniela Aparecida Chagas de Paula [1]

[1] Universidade Federal de Alfenas

The isolated substance from O. diospyrifolia showed to be an unpublished aporphine derivative. Anti-inflammatory activity of the substance isolated was evaluated and confirmed.

Obtention of δ-lactam through supercritical dioxide carbon extraction from Bunchosia glandulifera seeds.

https://proceedings.science/p/120718

Sara Fraga [1]; Fábio Domingues Nasário [1]; Anita Marsaioli [1]; Daniel Gonçalvez [1]; Larissa Ribas [1]; Klicia Araújo Sampaio [1]

[1] Universidade Estadual de Campinas

Use of a green extraction by supercritical CO2 technology to obtain caferana seed extracts.
Isolation, purification and characterization of δ-lactam, an uncommon and valuable product.

Optimization of extraction methods and chromatographic analysis of bee extracts for pesticide analysis

https://proceedings.science/p/120230

Maria Eduarda Constantini Teixeira [1]; Norberto Peporine Lopes [2]

[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP); [2] Universidade de São Paulo

Bees are pollinating agents that find in the nectar and pollen as their source of food and energy. They belong to the order Hymenoptera, of extreme importance for the conservation of plant and animal species, since they house the largest number of pollinators. Pollination is one of the most important mechanisms for maintaining biodiversity, and in

this scenario, according to the United Nations Food and Agriculture Organization (FAO), it is estimated that of the 100 species of crops responsible for providing 90% of the food in the world, 71 are pollinated by bees. In addition, bees are responsible for the production of honey and other supplies, such as wax and propolis, which contribute to human well-being. Since the 80's and 90's there has been a gradual reduction in the number of bees, but in a small magnitude. Currently, these insects are at high risk of extinction, and it is believed that a combination of several factors causes this population decline, such as deforestation, climatic variations, pathogens (viruses, bacteria, mites) and use of pesticides. Contamination of bees by pesticides can result from the negligent use of farmers, for example, by striking them for imagining that they harm the crop. Pesticide residues can be absorbed by bees during the collection of nectar and/or pollen and water. This project aims to seek the correlation between bee mortality and the use of pesticides, through modern chromatography techniques coupled with mass spectrometry, which will support the attainment of metabolic profiles subsidizing the search for pesticide residues in these bees. This because it is extremely important to assess the reach of pesticides in the environment and understand what impact they cause on bees and other pollinators. To achieve this proposed objective, several methods of extraction and analysis were selected in order to obtain the best methodology.

Optimization of ultrasound-assisted extraction of antioxidant compounds from Lantana camara Linn. leaves

https://proceedings.science/p/119694

Raphael Amancio de Jesus [1]; Pedro Ellison Santos do Nascimento [1]; Matheus Henrique Santos Santana [1]; Julio Manoel Andrade Oliveira [1]; Luís Fernando de Andrade Nascimento [1]; Arie Blank [1]; Paulo Nogueira [1]; Valéria Regina de Moraes [1]

[1] Universidade Federal de Sergipe

The extract from Lantana camara Linn. leaves obtained using the best condition by Ultrasound-Assisted Extraction displayed better antioxidant activity than the extract obtained by maceration.

Perfil Químico de Citrus Sinensis enxertada em Citrus Limonia por ferramentas quimioinformáticas e UPLC-Qtof-MS/MS

https://proceedings.science/p/120629

Fernanda Amaral Faria [1]; Luciano da Silva Pinto [1]; Maria Fatima das Gracas Fernandes Silva [2]

[1] Universidade Federal de São Carlos; [2] Departamento de Química, Universidade Federal de São Carlos

Influence of Citrus limonia rootstock on citriculture. Metabolomic analysis by mass spectrometry. GNPS platform for identification of secondary metabolites.

Perfil Químico e potencial bioherbicida do óleo essencial de Copaifera sp.

https://proceedings.science/p/120729

Marilene Oliveira [1]; Joseila Maldaner [1]; Simone Simote [1]; Darlisson de Alexandria Santos [2]; Fernanda dos S. Silva [1]; Maria Vitória da S. Meireles [1]; José Airton de S. Junior [1]; Sandy dos S. Rocha [1]; Selma Lopes Goulart [3]

[1] Universidade Federal do Sul e Sudeste do Pará; [2] Universidade do Sul e Sudeste do Pará; [3] Universidade Federal Rural da Amazônia

Copaiba hydrodistillation generated a yield of 7.9% essential oil (OE). The chemical characterization of OE was performed by CG-MS. The EO reduces lovegrass germination and growth.

Phenolic compound biotransformation by Trametes versicolor ATCC 200801 and molecular docking studies

https://proceedings.science/p/120031

Valmore Henrique Pereira dos Santos [1]; João Carlos Silva Conceição [1]; Herbert Júnior Dias [2]; Clarissa Maria Souza Peralva [1]; Antônio Eduardo Miller Crotti [2]; Eliane Silva [3]
[1] Universidade Federal da Bahia; [2] Universidade de São Paulo; [3] UFBA

Microbial biotransformation has become a tool of great importance in the modification of compounds for chemical, pharmaceutical and agrochemical industries, due to the high chemo-, regio- and stereoselectivity provided by the enzymes generated in situ. Laccases are oxidoreductase-type enzymes and occur in fungi, bacteria, and plants. Such enzymes are capable of oxidizing electron-rich substrates, including various phenolic compounds and aromatic amines. Laccases produced by Trametes versicolor (Tvlac) have one of the greatest redox potentials and constitute the main extracellular components of the fungus. The aim of the present study was to comprehensively evaluate the biotransformation of methyl p-coumarate (**1a**), methyl ferulate (**2a**), and methyl caffeate (**3a**) by *Trametes versicolor* ATCC 200801. For this, 5 mg of each substrate (**1a**, **2a** and **3a**) were solubilized in 350 µL of DMSO and added to Erlenmeyer flasks holding 50 mL of fermentation medium (0.2% glucose, 0.2% malt extract, 0.1% peptone, 0.1% Tween 80, 0.0005% copper (II) sulfate, pH 5.5), and five 6- mm disks containing mycelia. The biotransformation experiments were carried out at 28 °C for 72 h under stirring at 120 rpm. All the experiments were performed in triplicate. Samples were taken daily until the finish of the experiment. Additionally, molecular docking analysis was performed to study the interactions between the substrates with Tvlac active sites, by using the AutoDock v.4.2 software where the Lamarckian genetic algorithm (LGA) is implemented. The biotransformation results showed that only the substrate **1a** was derivatized under the evaluated conditions. The crude extracts of the biotransformations were analyzed by HPLC-DAD, indicating the formation of metabolites **1**, **1b** and **3a**. The molecular docking analysis showed different variations of Gibbs free energy (ΔG) for substrates **1a**, **2a** and **3a**, with values of -6.39, -7.37 and -7.55 kcal/mol, respectively. The lower ΔG value obtained for **1a** indicated greater reactivity (less stability) in comparison with **2a** and **3a**, justifying the formation of derivatives from **1a**. In summary, our results showed that the position and type of substituents in the aromatic ring of phenolic substrates influenced their conformation and orientation at the Tvlac site. Substrates that contained two substituents on the aromatic ring (methyl ferulate and methyl caffeate) displayed additional hydrogen-bonding interactions with Tvlac, which increased the stability of the Tvlac-substrate complexes and prevented the biotransformation occurrence.

Phenolic glycosides of Myrcia guianensis (Myrtaceae)

https://proceedings.science/p/120727

Cristhian Santos Oliveira [1]; Vanessa Winiewski [2]; Maria Élida Alves Stefanello [2]
[1] Química / Setor de Ciências Exatas / Universidade Federal do Paraná; [2] Universidade Federal do Paraná

Two known phenolic glycosides, lanceoloside A (1) and 6-O-galloylarbutin (2) were isolated from Myrcia guianensis leaves for the first time.

Phytochemical prospecting of banana peel biomass

https://proceedings.science/p/120215

Fabrícia dos Santos Leal [1]; SILVIO CUNHA [2]; Eliezer Silva [1]; Rodrigo de Paula [1]
[1] Universidade Federal do Recôncavo da Bahia; [2] Universidade Federal da Bahia

The objective of this work is to study the methods of extracting the banana peel. TLC, qualitative tests and HPLC-MS analyses were carried out to determine the chemical composition of major compounds.

Phytochemical prospecting of leaves and latex of Jatropha mollissima (Pohl) Baill

https://proceedings.science/p/120223

Jamilly Eli da Silva Rodrigues [1]
[1] Universidade Federal de Alagoas

The extracts of leaves and latex of Jatropha mollissima (Pohl) Baill were evaluated for chemical composition, dentifying the main secondary metabolites using a qualitative method.

Phytochemical prospection of Eugenia species (MYRTACEAE) leaves extracts

https://proceedings.science/p/120071

Beatriz Nascimento de Araujo [1]; Glauce C. A. Duarte [2]; Erika M. de Carvalho [3]; July A. H. Muñoz [3]
[1] Universidade Federal do Rio de Janeiro; [2] Universidade Federal Fluminesce; [3] FIOCRUZ

Results obtained from phytochemical prospection showed that Eugenia species may have different chemical classes. First report of the presence of barbinervic acid from species of E.florida .

Phytotoxic Activity and Phytochemical Study of Sphagneticola trilobata (L.) Pruski

https://proceedings.science/p/120740

Naomi Kato Simas [1]; Carina Morgado [1]; Anne Caroline Candido Gomes [2]
[1] Universidade Federal do Rio de Janeiro; [2] Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro

Allelochemicals have been identified in Sphagneticola trilobata. This species showed phytotoxic activity in the growth of L. sativa and I. purpuea seeds, being a possible alternative for weed control.

Polysaccharides of Pleurotus eryngii: extraction, purification and chemical characterization

https://proceedings.science/p/120737

Priscilla Duarte [1]; Dayane de Brito [1]; Ruberney da Silva de Oliveira [1]; Sthefany Rodrigues Fernandes Viana [1]; Maria Carolina Bezerra Di Medeiros Leal [2]; Elaine Rosechrer Carbonero [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal de São Carlos

- Macrofungi are important sources of bioactive substances;
- P. eryngii is an edible and medicinal mushroom;
- Unusual heteropolymers were isolated.

Preliminary analysis of the chromatographic profile of Colletotrichum sp. aiming at proposing chemical markers by pattern recognition.

https://proceedings.science/p/120050

Tatiane da Costa Lima [1]; Marilene Nunes Oliveira [2]; Licarion Pinto [3]; Alciene Lima dos Santos [2]; Adriano de Araujo Gomes [4]; Darlisson de Alexandria Santos [2]; Kézia Ferreira Alves [5]; Simone Yasue Simote Silva [2]; Sebastião da Cruz Silva [2]
[1] UNIVERSIDADE FEDERAL DO SUL E SUDESTE DO PARÁ-UNIFESSPA; [2] Universidade do Sul e Sudeste do Pará; [3] Universidade Federal de Pernambuco; [4] Universidade Federal do Rio Grande do Sul; [5] Instituto Federal de Castanhal

Extraction and characterization of Volatile Organic Compounds via HS-SPME / CG-MS. Pattern recognition analysis to identify chemotaxonomic markers.

Prospecção química da fração ativa de Bauhinia holophylla com potencial inibitório em arginase de Leishmania amazonensis.

https://proceedings.science/p/120708

Thais Bertolino Vieira Dantas [1]; Romário Pereira da Costa [2]; Dulce Helena Ferreira de Souza [2]; Quezia Bezerra Cass [2]; Richele Priscila Severino [3]; Lorena Ramos Freitas de Sousa [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal de São Carlos; [3] Universidade Federal de Catalão

Chemical prospection of stem bark of Bauhinia holophylla allowed to identify flavan-3-ols from active fraction with ARG inhibitory activity.

Pyrrolizidine alkaloids of two species of Crotalaria grown under conventional and in vitro conditions

https://proceedings.science/p/119590

Daiane Einhardt Blank [1]; Antonio Demuner [1]; Jilma Carvalho [1]; Gustavo Souza [1]; Maria Firmino [1]; Wagner Campos Otoni [1]; Daniele Faria [1]; Lorena Vieira [1]; Guilherme Zocolo [2]; Jhonyson Guedes [2]
[1] Universidade Federal de Viçosa; [2] Empresa Brasileira de Pesquisa Agropecuária

Pyrrolizidine alkaloids are markers for Crotalaria. In vitro culture was performed to obtain alkaloids and compare with conventional culture. Alkaloids were identified by UPLC-QTOF-MSE.

Regioselective Mannich aminomethylation of α-mangostin and D-proline: funcionalization of bioactive phenolics to their conjugation to peptide chains

https://proceedings.science/p/120732

Gabriella Calheiros Magalhães [1]; Marco Edilson Freire de Lima [1]; Paulo Pitasse [1]; Gabriela de Souza [1]; Douglas Chaves de Alcantara Pinto [1]
[1] Universidade Federal Rural do Rio de Janeiro

Regioselective functionalization of natural xanthone α-mangostin isolated from G. mangostana with D-proline through
Mannich reaction. Solid-supported synthesis of peptide-drug conjugate.

Secondary metabolism and cytotoxic effects of Penicillium setosum, an unknown fungus obtained from Swinglea glutinosa

https://proceedings.science/p/120706

Ana Carvalho [1]; Cauê Lima [1]; Heron Fernandes Vieira Torquato [1]; Edgar Paredes-Gamero [2]; Lívia Soman [1]; THIAGO VEIGA [1]
[1] Universidade Federal de São Paulo; [2] Faculty of Pharmaceutical Sciences, Food and Nutrition - Federal University of Mato Grosso do Sul – UFMS, Brazil

Penicillium setosum, an unknown endophytic fungus is being studied in this work. The crude extract, its fractions and a purified compound presented cytotoxic effects against human leukemia cell lines.

Secondary metabolites from Annona sylvatica

https://proceedings.science/p/120393

Lúcia Pinheiro Santos Pimenta [1]
[1] Universidade Federal de Minas Gerais

Sesqui and diterpene identified from the hexane phase of Duguetia lanceolata (Annonaceae) and evaluation of antileishmanial activity.

https://proceedings.science/p/119971

Jackson Monteiro [1]; Luiz Felipe Domingues Passero [2]; João Henrique Ghilardi Lago [3]; Patricia Sartorelli [1]
[1] Universidade Federal de São Paulo; [2] Universidade de São Paulo; [3] Universidade Federal do ABC

The chromatographic fractionation of the hexanic phase of the leaves of D. lanceolata. Bioguided fractionation by antileishmanial activity. Identification by spectroscopic analysis of NMR and by GC-MS

Síntese, Caracterização e Aplicação de Novos Meios de Alinhamento para Medidas Anisotrópicas de RMN

https://proceedings.science/p/120307

Fernando Hallwass [1]; Cleyton Marcos de Melo Sousa [2]; Daiane de Souza Carvalho [1]; Danilo Gleibson Bernardo da Silva [1]; Gabriela Cavalvanti [1]; Higor Melo [1]; José Adonias de Franca [1]; Armando Navarro-Vásquez [1]

[1] Universidade Federal de Pernambuco; [2] Instituto Federal de Pernambuco

New polymer gels, chromonic liquid crystals, and graphene-based mesophases, were prepared as weakly aligning media for the obtaining RDC and RCSA data in different solvents

Study of secondary metabolites in different coculture methodologies among microorganisms present in leaf-cutting ant nests

https://proceedings.science/p/120728

Joao Batista Fernandes [1]; Dorai Zandonai [1]; Alana Kelyene Pereira [1]; Maria Fatima das Gracas Fernandes Silva [2]; Moacir Forim [1]

[1] Universidade Federal de São Carlos; [2] Departamento de Química, Universidade Federal de São Carlos

The work aims to control the mutualistic fungus, Leucoagaricus. gongylophorus, and as a consequence leaf-cutting ants, through cocultivations in different approaches to induce metabolites.

STUDY OF THE ANTIOXIDANT POTENTIAL OF BURITI (Mauritia Flexuosa L.f.) EXTRACTS IN VEGETABLE OILS

https://proceedings.science/p/120297

Vanessa Albuquerque de Mescouto [1]; Rayanne Danielle dos Reis Gonçalves [2]; Maitê Campos [2]; Larissa Gatti [2]; Aimée Souza da Silva [2]; Samantha Siqueira Pantoja [2]; Luiza Helena de Oliveira Pires [2]; GERALDO Narciso da Rocha Filho [2]; Luis Adriano Santos do Nascimento [2]

[1] UFPA (Universidade Federal do Pará); [2] Universidade Federal do Pará

Buriti pulp was investigated as a source of natural antioxidants. The effects of buriti pulp extracts in the Brazil nut and in the passion fruit oils were evaluated.

TRIAGEM FITOQUÍMICA E POTENCIAL ALELOPÁTICO DE Ocimum gratissimum

https://proceedings.science/p/119722

Elieuda dos Reis Santos [1]; Darc Barbosa [2]; Alessandra Ramos [3]; Tatiani Luz Silva [3]

[1] Universidade do Estado do Pará--Campos VIII/Marabá ; [2] Universidade do Estado do Pará (UEPA); [3] Universidade Federal do Sul e Sudeste do Pará

O Ocimum gratíssimum lamiaceae é um vegetal de origem asiática e muito conhecida e utilizada na culinaria brasileira e para tratamento de várias doenças, foram realizados os testes fitoquímicos e alelopático afim de identificar as classes de substâncias presentes no extrato hidroalcóolico da planta e verificar o potencial alelopático frente a sementes de Lactuca sativa.Os resultados foram satisfatório porem há a necessidade de novos testes com substancias isoladas da planta para comprovação dos resultados.

Triterpenos e esteroides isolados de Oeceoclades maculata (Orchidaceae) e avaliação da atividade citotóxica contra células VERO e HeLa

https://proceedings.science/p/120716

Paula Cristina Perin [1]; Silvana M. de Oliveira Santin [1]; Maria A. Milaneze-Gutierre [1]; Beatriz V. Diniz [1]; Melyssa F. N. Negri [1]; Armando M. Pomini [1]

[1] Universidade Estadual de Maringá

Chemical study of the O. maculata afforded two triterpenes and three steroids. Compounds were identified by their spectral data. Crude extract and fractions were evaluated against VERO and HeLa cells.

UMBELLIFERONE ESTERS WITH ANTIBACTERIAL ACTIVITY PRODUCED BY BIOCATALYTIC PATHWAYS

https://proceedings.science/p/120792

Vitor Soares [1]; Larissa Assis de Paula [2]; Rafael Viana Calazans Maia [2]; Maíra Barcellos Marini [2]; Marcelo Mignoni [3]; Camila Adão Malafaia [2]; Ivana Correa Ramos Leal [2]

[1] Instituto Federal do Paraná - IFPR; [2] Universidade Federal do Rio de Janeiro; [3] URI Erechim

Coumarins and their derivatives comprise an important class of secondary metabolites produced by a large range of plant sources. Literature reports different types of biological activities for these compounds and among them are the antimicrobial, anticoagulant, estrogenic, anti-inflammatory, anti-HIV, antioxidant, and other. As promising therapeutic agents, new and sustainable methodologies for those synthesis may gain even more prominence with a green and lower cost approach [1,2]. So, the derivatization of a coumarin skeleton can improve the activity as already observed in literature for other phenolic compound, such as flavonoids. The present report describes the enzymatic acylation of umbelliferone with different vinyl esters as acyl donors biocatalyzed by the commercial lipase Novozym® 435 and by an endophytic fungi immobilized in zeolite. It also aims the investigation for their antibacterial activity against ATCC and clinical strains isolated from hospital infection sites. The umbelliferone esters (1—5) were synthesized through the acylation reaction of 7-hydroxy-2H-chromen-2-one with different long chain vinyl esters catalyzed by the lipase Novozym 435. The reaction conditions were: 10 % Novozym 435; tetrahydrofuran:acetone (3 (solvent):1(cosolvent)) for the reactions with acetate, propionate and butyrate vinyl esters, and (9 (solvent):1(co-solvent)) for decanoate and laurate vinyl esters; acyl donor /umbelliferone molar ratio of 10:1 and 60 °C. Aliquots (20 µL) were withdrawn from 24 to 168 h and analyzed by GC-MS. All tumbelliferone esters were characterized by Nuclear Magnetic Resonance (NMR) and high resolution mass spectrometry (HRMS). The recycle of the reactions will be evaluated for both biocatalysts. The esters with short chain achieved 50—90 % conversion while with the long chain vinyl esters achieved 10 – 15 % conversion. The antibacterial activity of the products were tested in order to determine the minimum inhibitory concentration (MIC) against ATCC strains (S. aureus ATCC 33591 and ATCC 29213; S. epidermidis ATCC 12228; S. hominis ATCC 27844; S. simulans ATCC 27851; S. saprophyticus ATCC 15305; Pseudomonas aeruginosa ATCC 27853; Klebsiella pneumoniae ATCC 700603; E. coli ATCC 25922) and clinical strains (CS) (S. aureus CS 601, CS 664, CS527, CS 551, CS 517 CS 1025; Acinetobacter spp. CS OXA-51; A. baumannii CS 55a). The results displayed by 7-laurate and 7-decanoate-umbelliferone esters showed the highest antibacterial potential, with 1 mM inhibitory activity for ATCC 33591, a methicillin and oxacillin resistant Staphylococcus aureus strain. They were also able to inhibit gram-negative bacterial strains, such as P. aeruginosa (MIC: 0.5 mM) and K. pneumoniae (MIC:1 mM). In addition, 7-laurate- and 7-decanoate-umbelliferone esters were able to inhibit all clinical strains (MIC: 1mM; except 7-laurate-umbelliferone in which MIC: 0.5 mM against 55a). The reactions with the endophytic fungi immobilized in zeolite (rich in lipases) will be also conducted and the conversion rates established. This is the first study performing the biocatalysis of umbelliferone followed by the purification of the products and the antibacterial evaluation.

Use of ionic liquid in the microwave assisted extraction of new butanolides with in vitro antiparasitic activity from Nectandra barbellata (Lauraceae) twigs

https://proceedings.science/p/120053

Vinicius Silva Londero [1]; Guilherme Antar [2]; João Baitello [3]; Thais Costa-Silva [4]; André Gustavo Tempone [5]; Larissa Verena Figueiredo de Oliveira [1]; Fernanda Ferraz Camilo [1]; João Henrique Ghilardi Lago [6]

[1] Universidade Federal de São Paulo; [2] Universidade de São Paulo; [3] Instituto Florestal-Secretaria de Infraestrutura e Meio Ambiente do Estado de São Paulo; [4] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC; [5] Adolfo Lutz; [6] Universidade Federal do ABC

This work reports the use of ionic liquid in the microwave assisted extraction (MAE) of three new related butanolides (1 – 3) from twigs of Nectandra barbellata (Lauraceae) with antiparasitic activity

Using GNPS tools to accelerate the metabolites identification of complex marine bacterial extracts.
https://proceedings.science/p/119615

Eduarda A. Moreira [1]; Anelize Bauermeister [1]; Paula Rezende-Teixeira [2]; Leticia Lotufo [1]; Norberto Lopes [1]
[1] Universidade de São Paulo; [2] University of Sao Paulo

GNPS tools annotated diverse marine bacterial metabolites, supporting a faster and more reliable dereplication process. The annotations included β-carbolines, lipopeptides, bile acids and carbazoles.

Uso de ferramentas de quimioinformática e mineração de dados com objetivo de compreender a atividade antimicrobiana de isoflavonas
https://proceedings.science/p/119879

Juliane Xavier dos Santos [1]; Nicholas J. Sadgrove [2]; Gugulethu Khumalo [3]; Ben-Erik van Wyk [3]; Tiago Branquinho Oliveira [1]
[1] Universidade Federal de Sergipe; [2] Royal Botanic Gardens, Kew; [3] University of Johannesburg

This work developed a QSAR study able to predict potentially inhibitory isoflavones for Staphylococcus aureus.

Xanthones of Phomopsis sp., an endophytic fungus obtained from Baccharis oxyodonta DC. (Asteraceae)
https://proceedings.science/p/120353

Eunizinis S. Kawafune [1]; Juliana C. S. Carvalho [1]; Oriana A. Fávero [2]; Paulete Romoff [2]; Marcelo J. P. Ferreira [1]; Marcelo J. P. Ferreira [1]
[1] USP; [2] Universidade Mackenzie
Few studies were carried out about endophytic fungi from Baccharis (Asteraceae).Three xanthones were identified of *Phomopsis* sp.

Química Ambiental - AMB

ANÁLISE DA COMPOSIÇÃO DO PERIFÍTON OBTIDO EM ALGAL TURF SCRUBBER SOBRE DIFERENTES CONCENTRAÇÕES DE NUTRIENTES
https://proceedings.science/p/120414

Rosana Schneider [1]; Tiele Medianeira Rizzetti [1]; Mateus da Silva Szarblewski [1]; Gisele Alves [1]; Michele Hoeltz [1]; Lisianne Brittes Benitez [1]
[1] Universidade de Santa Cruz do Sul

Evaluate the behavior of an ATS system in laboratory-scale.
Biomass productivity with NPK nutrient.
The lipid content was 9.6 ± 1.45% (w/w).
Periphyton identification in the bioremediation system.

ANÁLISE DA CONTAMINAÇÃO GEOGÊNICA EM ÁGUAS SUBTERRÂNEAS NA REGIÃO DO NOVO AIRÃO, ESTADO DO AMAZONAS

https://proceedings.science/p/120641

Tereza Cristina Souza de Oliveira [1]; Amanda O. Ribeiro [1]; Ingo D. Wahnfried [1]
[1] Universidade Federal do Amazonas

Two thirds of urban centers in amazon region uses underground water as main source of supply, and riverine communities were never object of research about the presence of water contaminants.

Análise da contribuição veicular e industrial aos níveis de ozônio e a qualidade do ar durante o lockdown parcial no Rio de Janeiro.

https://proceedings.science/p/120439

Guilherme de Sousa Dantas [1]; Bruno Siciliano Ramos Barros [1]; Bruno Bôscaro França [2]; Graciela Arbilla de Klachquin [1]; Cleyton Martins da Silva [3]
[1] Universidade Federal do Rio de Janeiro; [2] Secretaria Municipal do Meio Ambiente Rio de Janeiro; [3] Universidade Veiga de Almeida

Increased ozone levels during COVID-19 partial lockdown.
Reduced NOx levels under VOC-limited conditions.
Increased NMHC/NOx in industrial impacted areas.

Análise de hidrocarbonetos (C2-C12) usando cromatografia a gás multidimensional de corte sem criogenia.

https://proceedings.science/p/120441

Bruno Siciliano Ramos Barros [1]; Cleyton Martins da Silva [2]; Graciela Arbilla de Klachquin [1]
[1] Universidade Federal do Rio de Janeiro; [2] Universidade Veiga de Almeida

C2-C12 analysis without cryogenic cooling.
Extended hydrocarbon analysis in environmental and vehicular emission samples.
Thermal desorption, flame ionization and mass spectrometry detection methods.

Aplicação de análises clássicas para o estudo de sedimentos do Porto de Suape no Cabo de Santo Agostinho, estado de Pernambuco

https://proceedings.science/p/120035

Rayane Nascimento [1]; Ana Flávia B. de Oliveira [2]; Bruna Ramos de Souza Gomes [2]; Alex Souza Moraes [3]; Jandyson Santos [3]
[1] Universidade Federal Rural de Pernambuco (UFRPE)/ Programa de Iniciação Científica, Departamento de Química.; [2] Universidade Federal Rural de Pernambuco (UFRPE)/ Programa de Pós-Graduação em Química, Departamento de Química.; [3] Universidade Federal Rural de Pernambuco (UFRPE)

A contaminação de ambientes aquáticos tem sido um dos maiores problemas enfrentados pela sociedade. Em vários países as atividades portuárias estão se desenvolvendo rapidamente, exigindo maior atenção, principalmente no que diz respeito a gestão ambiental.1 Assim, ambientes costeiros e marinhos recebem grande quantidade de descargas de atividades humanas e industriais. Atualmente, existem poucos estudos científicos voltados para a caracterização química de amostras ambientais provenientes de complexos portuários visando o monitoramento ambiental dessas áreas. O estudo aqui descrito tem o objetivo de realizar a caracterização de amostras de sedimentos a partir da aplicação de análises clássicas em amostras coletadas no Porto de Suape, localizado no estado de Pernambuco. O Complexo Portuário de Suape abrange cerca de 100 empresas, em diferentes áreas de atuação, entre elas, atividades vinculadas a cadeia do petróleo e a presença de estaleiros, com a função de construir e reparar navios e embarcações. Na região do Porto, devido à dificuldade de autorização e acesso, foi conseguido a coleta de 5 amostras de sedimentos (códigos P1-P5) em diferentes áreas, na sua porção superficial (0-10 cm) com o auxílio de uma draga de Van Veen. As amostras passaram pelos processos de secagem em estufa de circulação a 60 °C por 48 h, seguidas de pulverização com pistilo e peneiramento com peneira de aço inoxidável (≈2 mm). Aos sedimentos, foram aplicadas as análises

clássicas: análise elementar (após a descarbonatação dos sedimentos com HCl), espectroscopia no infravermelho por transformada de Fourier com reflectância total atenuada (FTIR-ATR), análise granulométrica (frações de areia, silte e argila) e teor de matéria orgânica (realizado em mufla a 750 °C/6 horas), visando obter a caracterização preliminar das amostras em estudo. Como normalmente ocorre para este tipo de matriz, os espectros de FTIR-ATR apresentaram picos característicos de materiais argilosos, silicatos e ácidos húmicos, porém, pôde-se observar interessantes picos entre 2920-2850 cm- [1], características do estiramento assimétrico e simétrico -CH3 e -CH2 referente a hidrocarbonetos alifáticos. Esses picos podem estar associados a níveis de contaminação por petróleo[2] e se destacaram nos pontos de amostragem P1, P2 e P5, localizados próximos as atividades dos estaleiros e da área de carga/descarga de petróleo e gás do Porto, o que sugere uma possível contaminação por hidrocarbonetos nestas regiões. A partir da análise granulométrica, observou-se que as amostras localizadas próximas aos estaleiros (P1 e P2) são compostas majoritariamente por partículas finas, e consequentemente maior percentual de matéria orgânica, assim, associamos essa característica ao processo de dragagem realizado nesses pontos a fim de assegurar a profundidade do canal para o acesso de grandes embarcações. Todos os pontos de coleta apresentaram valores da razão TOC/TN superior a 15, que indica contaminação por esgoto, devido a entrada de carbono por fontes antropogênicas[3]. Os resultados desse estudo mostram a caracterização química de sedimentos do Porto de Suape a partir da aplicação de análises clássicas, dando informações preliminares a respeito das características dos sedimentos, onde alguns dados apontam para a existência de regiões com indicativo de contaminação antropogênica. Como perspectiva, a identificação e quantificação de marcadores ambientais da classe dos hidrocarbonetos alifáticos e policíclicos aromáticos pode ser uma alternativa para a confirmação dos indicativos de contaminação obtidos em nosso estudo.

Aplicação do rejeito de mineração no processo de fotodegradação do pesticida tiabendazol

https://proceedings.science/p/120621

Tainara Ramos Neves [1]; Barbara Queiroz Guimarães [1]; Lucas Lorenzini [1]; Ana Caroline Silva de Campos [1]; Maria de Fátima Fontes Lelis [1]; Sandra Aparecida Duarte Ferreira [1]
[1] Universidade Federal do Espírito Santo

Reuse of mining tailing. Ferrite Synthesis. Wastewater treatment

Avaliação do aporte e perfil isotópico de carbono em n-alcanos em sedimentos lacustres do Lago Comprido, Amazônia brasileira.

https://proceedings.science/p/120378

Karoline Ribeiro dos Santos [1]; Alexander A. Lopes [2]; Vinicius Barreto Pereira [2]; Raquel Viera Santana da Silva [2]; Débora de Almeida Azevedo [2]
[1] Universidade Federal Do Rio de Janeiro; [2] Universidade Federal do Rio de Janeiro

Geochemical assessment of the origin of organic matter sediment core from the Brazilian Amazon using n-alkane proxies and isotopic composition

BeeToxAI: Um Portal Online Baseado em Inteligência Artificial para Predizer a Toxicidade Aguda de Produtos Químicos em Abelhas Melíferas

https://proceedings.science/p/120542

José Teófilo Moreira-Filho [1]; Rodolpho Braga [2]; Joyce Borba [1]; Eugene N Muratov [3]; Carolina Andrade [1]; Bruno Neves [4]

[1] LabMol – Laboratory for Molecular Modeling and Drug Design, Faculty of Pharmacy, Universidade Federal de Goiás, Goiás, 74605-170, Brazil; [2] InsilicAll Inc., São Paulo, 04363-090, Brazil; [3] Laboratory for Molecular Modeling, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, North Carolina, 58059-900, USA; [4] Universidade Federal de Goiás

The use of pesticides has been associated with the drastic decline of bee populations in several countries. Honey bee species such as Apis mellifera are of utmost importance because of their vital ecological duty as pollinators of wild plants and crops. Consequently, scientific advisory bodies have standardized in vivo protocols to access acute toxicity of chemicals in honey bees. In view of the costly and time-consuming characteristics of experimental assays, we developed an innovative artificial intelligence-based web portal to access acute toxicity of chemicals in honey bees.

Initially, we have collected and curated the largest publicly available dataset of compounds with acute contact and oral toxicity for A. mellifera. Then, 40 machine learning (ML) models were built using contact and oral datasets to distinguish toxic (LD50 ≤11 µg/bee) vs. non-toxic (LD50 >11 µg/bee) compounds. The model built using FeatMorgan_2 fingerprint + Random Forest demonstrated the best external predictivity among all other models developed for acute contact toxicity (ACC = 92%; SE = 83%; SP = 96%; and MCC = 81%). The model built using MACCS fingerprints + Support Vector Machine shown the best external predictivity among all other models developed for acute oral toxicity (ACC = 91%; SE = 93%; SP = 93%; and MCC = 82%). These models are freely available through the BeeToxAI web portal at http://beetoxai.labmol.com.br/. The BeeToxAI (Figure 1) allows users for fast screening of compounds. After drawing or importing a molecule and submitting it to a prediction, the user will receive in few seconds the predicted outcomes for acute contact and oral toxicities. These predictions are followed by probability estimates, which are useful for estimating the confidence of predicted outcomes, the applicability domain estimates, and mechanistic interpretation of prediction using contribution maps (atoms with positive and negative contributions for toxicity). In summary, BeeToxAI can be used as a reliable alternative to animal tests for predicting acute toxicity of chemicals in honey bees.

Bioavailability and risk assessment of potentially toxic metals in sediments of Paraibuna River (Juiz de Fora, MG) based on SEM-AVS analysis

https://proceedings.science/p/120218

Ricardo Soares [1]; Angela Sanches Rocha [2]; Wilson Machado [3]; David Vilas Boas de Campos [4]; Maria Inês Monteiro [5]; Aline Soares [6]; Ricardo Santelli [6]

[1] INEA; [2] UNIVERSIDADE DO ESTADO DO RIO DE JANEIRO; [3] Universidade Federal Fluminense; [4] Empresa Brasileira de Pesquisa Agropecuária; [5] Centro de Tecnologia Mineral; [6] Universidade Federal do Rio de Janeiro

The levels of AVS were much less variable than SEM in all sediment samples.
AVS have not acted as an important carrier for SEM in sediments of Paraibuna River
The levels of SEM were Zn>Ni>Cu>Pb>Cd.

Biosorption Kinetics of Organic Dye in Crustaceans Residues Found in the State of Sergipe

https://proceedings.science/p/120363

Jefferson Arlen Freitas [1]; Victor C.s. Freire [1]; Ellen Barbosa Nunes Góes [2]; André Augusto Fonseca Ferreira [2]; José Jailton Marques [1]; Roberto Rodrigues de Souza [3]; Eliana Sussuchi [4]

[1] Universidade Federal de Sergipe/Departamento de Engenharia Ambiental/Laboratório de Tecnologias Ambientais-LATAM/DEAM/UFS; [2] Universidade Federal de Sergipe/Departamento de Engenharia Química/Laboratório de Biotecnologia Ambiental-LABAM/DEQ/UFS; [3] Universidade Federal de Sergipe, Departamento de Engenharia Química, Laboratório de Biotecnologia Ambiental (LABAM/DEQ/UFS); [4] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS)

Removal of the organic dye of effluents with crustaceans residues. Fast kinetics of biosorption of methylene blue in crustacean residues adjusted well to the pseudo-second order model.

Calibração de BTX por cromatografia gasosa através de headspace dinâmico

https://proceedings.science/p/120449

Laurênio Ferreira Lopes [1]

[1] Universidade Federal Fluminense

BTX calibration by gas chromatography using dynamic headspace. Air pollution is composed of volatile organic compounds, with benzene being the most health-damaging species.

Caracterização química e comparação entre as bacias do Rio doce e Santo Antônio após o rompimento da Barragem de Fundão

https://proceedings.science/p/120386

Claudia Windmöller

Characterization of asbestos fibers in the soil and proven rainwater from fiber cement tiles

https://proceedings.science/p/119853

Lincoln Gabriel Santiago de Aquino [1]; Danielle C. Schnitzler
[1] Universidade Técnológica Federal do Paraná

Asbestos is a mineral fiber used in the industry due to its resistance characteristics that are given to the materials that use it; Systems were set up in the environment, with rain and soil water being collected analyzing the possible release of asbestos fibers from fiber cement tiles. It was possible to notice that samples of older tiles release a greater number of fibers in the environment.

Characterization of the organic fraction of urban-coastal particulate matter (PM2.5 and PM10)

https://proceedings.science/p/119852

Elizanne Porto de Sousa Justo [1]; Carlos German Massone [1]; Adriana Gioda [2]
[1] Departamento de Química / CTC / Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio); [2] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio)

Total PAHs were determined in PM using GC-MS.
PM10 exceeded the annual limit by WHO.
Majority 16 PAHs are attributed to vehicular emissions.

Chemical and toxicological assessment during chloramphenicol degradation in aqueous matrices by photolysis and heterogeneous photocatalysis

https://proceedings.science/p/119617

Alam Gustavo Trovó [1]; Eduardo Marson [1]; Cleiseano Emanuel da Silva Paniagua [2]; Raquel Maria Ferreira Sousa [1]; Gizele Damaceno Silva [1]; Raquel Wielens Becker [3]; Carla Sirtori [3]; Solidônio Rodrigues Carvalho [1]
[1] Universidade Federal de Uberlândia; [2] Universidade Federal de Uberlândia ; [3] Universidade Federal do Rio Grande do Sul

Chloramphenicol is an effective antibiotic for the treatment of gram-positive and gram-negative bacteria, and it has been frequently detected at concentrations between 0.0058 and 15.6 µg L-1 in different aqueous matrices around the world. In an attempt to reduce the contamination by chloramphenicol in the aquatic environment, new technologies should be evaluated as alternatives for removal and/or degradation of this contaminant. Therefore, photolysis and heterogeneous photocatalysis were evaluated for chloramphenicol degradation in deionized water (DW) and in a sewage treatment plant (STP) effluent under black light and solar radiation, and the processes were compared in terms of rate constants, electrical energy per order and theoretical prediction of toxicity, biodegradability, carcinogenicity and mutagenicity. An expressive difference in rate constants of chloramphenicol was observed in DW under photolysis and heterogeneous photocatalysis, but not in STP effluent as a consequence of the generation of photo-active reactive oxygen species (HO· and HO2·-/O2·-) under photolysis, as verified by experiments in the presence of trapping agents (2-propanol and chloroform). In addition, natural organic matter and HCO3- ions were the main factors responsible for the reduction of degradation rates of chloramphenicol in STP effluent. Fifteen transformation products of chloramphenicol were identified in DW under photolysis and heterogeneous photocatalysis, thirteen of which were reported for the first time. A degradation mechanism involving these compounds identified by both processes is presented, with the main pathway of chloramphenicol degradation being by preferential attack of HO· on the aromatic ring and its a-carbon. Additionally, predicted biodegradability and toxicological risk of the main identified transformation products could be classifying these compounds as persistent, toxic and as those that indicated potential genotoxicity or carcinogenicity. Finally, the use of sunlight can be considered a good alternative for treatment of water containing this pollutant, since it eliminates energy costs related to the radiation source.

CHEMOMETRIC INVESTIGATION OF THE SOIL DISPERSION PROFILE OF SOME CEPHALOSPORINS

https://proceedings.science/p/120264

André Mauricio de Oliveira [1]; Isabela B.S. Martins [1]; Larissa S. Santos [1]; Nicoly C. Garcia [1]; Luana C. Corrêa [1]; Roberto M. Glória [1]; Taíza P. B. Lucas [1]

[1] CEFET-MG

The ADMET study of some cephalosporins suggests a significant soil retention and low tendency to water leaching. Cephalosporins present a long range lipophilicity spectra due to their polar surfaces and substitution pattern. Soil persistence of these compounds depends on the overall lipophilicity.

Comparative study of the products from the pyrolysis of raw and hydrolysed Baru wastes

https://proceedings.science/p/119866

Magale Karine Diel Rambo [1]

[1] UFT

Physical/chemical characterization of Baru (Dipteryx alata Vog.), mesocarp and endocarp residue.> Pyrolysis process for converting biomass into biochar and bio-oil.> Characterization of biochars regarding the values of surface area (BET and LAGMUIR) and volume of micropores.> Potential application of this biomass in the context of biorefineries.

Comparison of pharmaceuticals degradation in surface water advanced oxidation processes

https://proceedings.science/p/119467

Cleiseano Emanuel da Silva Paniagua [1]; Vinícius Alexandre Borges Paiva [2]; Ivo Amildon Ricardo [2]; Eduardo Marson [2]; Bárbara Rezende Gonçalves [2]; Alam Gustavo Trovó [2]

[1] Universidade Federal de Uberlândia ; [2] Universidade Federal de Uberlândia

Pharmaceuticals are not removed by conventional processes, being determined in different aqueous matrices. Therefore, in this study the simultaneous degradation of gemfibrozil (GEM), hydrochlorothiazide (HCTZ) and naproxen (NAP) in surface water by advanced oxidation processes was evaluated. As can be seen in Table 1, high values of rate constants (k) and lower values of half-life time (t1/2) were obtained using the photo-Fenton process (FeOx/H2O2/UV-A) followed by photoperoxidation (H2O2/UV-C) and heterogeneous photocatalysis (TiO2/H2O2/UV-A). The t1/2 for the photo-Fenton process was, on average, sixteen (GEM), six (HCTZ) and nine (NAP) times shorter than the other processes evaluated. Moreover, it presented the lowest treatment cost per m3 of contaminated water, considering the reduction of the initial concentration of each compound by an order of magnitude. Thus, the photo-Fenton process may be used as an alternative of treatment for the removal of such contaminants. Table 1. Kinetic parameters obtained during the pharmaceuticals degradation by different advanced oxidation processes under optimized conditions. Initial conditions: [GEM] = [HCTZ] = [NAP] = 1.8 µmol L–1; pH 6.0. Processes Compounds Fe3+ (mg L-1) C2O42- (mg L-1) TiO2 (mg L-1) H2O2 (mg L-1) k (min-1) R2 t1/2 (min) Cost (R$) FeOx/H2O2/UV-A GEM 3.0 1.2 - 4 0.42 0.99 1.7 HCTZ 3.0 1.2 - 4 0.20 0.94 3.4 47 NAP 3.0 1.2 - 4 0.61 0.99 1.1 TiO2/UV-A GEM - - - - 0.0029 0.98 239 6402 - - 150 - 0.020 0.93 34 - - 150 6 0.039 0.96 18 HCTZ - - - - 0.0029 0.89 240 - - 150 - 0.012 0.98 58 - - 150 6 0.020 0.98 35 NAP - - - - 0.0028 0.92 250 - - 150 - 0.020 0.99 34 - - 150 6 0.045 0.92 15 H2O2/UV-C GEM - - - - 0.038 0.99 18 181 - - - 4 0.056 0.92 12 HCTZ - - - - 0.11 0.99 6.3 - - - 4 0.21 0.98 3.3 NAP - - - - 0.099 0.99 6.9 - - - 4 0.19 0.99 4.3

Contaminantes emergentes no Ribeirão das Pedras: o impacto desde a nascente até a foz

https://proceedings.science/p/119837

Juliana Sanchez Xavier dos Anjos [1]; Cassiana Carolina Montagner [1]

[1] Universidade Estadual de Campinas

The objective of this work is to monitor the presence of emerging contaminants in this water body and to evaluate the water quality seasonally along its extension.

Determinação de compostos orgânicos voláteis e estudo da qualidade do ar no bairro de Irajá, Rio de Janeiro.

https://proceedings.science/p/120044

Guilherme de Sousa Dantas [1]; Graciela Arbilla de Klachquin [1]; Cleyton Martins da Silva [2]
[1] Universidade Federal do Rio de Janeiro; [2] Universidade Veiga de Almeida

Coleta de compostos orgânicos voláteis no bairro de Irajá utilizando os métodos TO-15 e TO-11A. Os compostos mais abundantes forma alcanos, mas os aromáticos apresentaram maior reatividades cinética e mecanística formadora de ozônio. Todas as amostras de benzeno e etilbenzeno apresentaram concentrações maiores que os limites estipulados pela Agência de Proteção Ambiental dos EUA. A forte correlação entre COV/NOx e as concentrações e ozônio sugerem a necessidade de monitoramento contínuo destes poluentes.

Development of a protocol for simultaneous determination of microplastics and metals in fish tissue: an efficient way for monitoring environmental impact

https://proceedings.science/p/119884

Cezar Bizzi [1]
[1] UFSM

Distribuição de mercúrio total em água e sedimentos ao longo da Bacia Rio Reis Magos no Espírito Santo - Brasil

https://proceedings.science/p/120539

Eldis Sartori [1]; Sonara Gonçalves Silva Cassa [1]; Guilherme Yacovenco [1]; Madeline Jean Simon [1]; Maria Tereza Carneiro [2]; Geisamanda Pedrini Brandão [1]
[1] UFES (Universidade Federal do Espírito Santo); [2] UFES

The risk of Hg pollution in aquatic ecosystems. Sediment samples can be potencial sources of Hg. The highest concentrations of total Hg are associated with the highest content of organic matter.

Efficient removal of hexavalent chromium by in natura and magnetic nanomodified yeast biomass

https://proceedings.science/p/119818

Julia Cristina José [1]; Geórgia Labuto [2]; Elma N. V. M. Carrilho [1]
[1] Universidade Federal de São Carlos; [2] Universidade Federal de São Paulo, campus Diadema

Biosorption is one of the most attractive techniques for removing metal ions present in effluents using biological residues such as yeasts, which are generated in large quantities by fermentation industries and, in addition, have active sites for the adsorption of contaminants. Thus, this work proposed the use of in natura yeast biomass (YB) and a YB and Fe3O4 composite (YB-MNP) as biosorbents to remove Cr(VI) from water, considering that the superparamagnetic properties conferred to MNP facilitate the removal of material after the sorption process. The synthesis of MNP and YB-MNP was performed using the coprecipitation method for its application as an adsorbent material, and also as a modification of yeast biomass in order to compare the magnetization effect. Therefore, the use of the composite (YB-MNP) is a low cost and environmentally favorable alternative. All materials were morphologically characterized by FTIR to identify functional groups (C-C, C-H, O-H, N-H, C=O, etc.) and the Fe-O bond characteristic of magnetite, as well as to evaluate the efficiency of the composite synthesis. The adsorbents MNP and YB-MNP were analyzed by XRD and the results were compared to the characteristic crystalline planes of magnetite. All materials were also characterized by SEM to investigate the materials surface and to determine the chemical elements present and their respective proportions. Besides that, pHPZC was determined to define the pH at which the surface charge of the materials is positive or negative and contributes to a better Cr(VI) sorption capacity. The pHPZC determined for YB and YB-MNP was 5.7 and 6.0, respectively. Thus, initially, studies were carried out to remove Cr(VI) at lower pHs, since Cr(VI) is found mainly in the form of HCrO4 – ions. Thus, the pH was optimized to 2.0, where the removal of Cr(VI) was 4.61 mg/g (YB), 2.86 mg/g (MNP) and 4.03 mg/g (YB-MNP). Kinetic studies showed that equilibrium was obtained in the first 10 min (YB and YB-MNP) and 90 min (MNP), in which the sorption of Cr(VI) remained practically constant. In addition, the experimental sorption capacity of Cr(VI) by the materials used (YB, YB-MNP and MNP) was evaluated using the Freundlich, Sips, Dubinin Radushkevich (D-R), and Temkin isotherm models. Thus, it is noted that the

adsorption of Cr(VI) mainly by YB and YB-MNP is a promising procedure to potentially decontaminate effluents containing toxic metals.

Efficient Solid-Phase Extraction Of Diclofenac From Aqueous Solution Using Macrostructure Of Reduced Graphene Oxide

https://proceedings.science/p/119717

Raimara de Souza Gomes

Electrochemical degradation of Estradiol using a full factorial design associated with diamond electrodes

https://proceedings.science/p/120352

Calixto Fernandes Filho [1]; Thays Lima [2]; Letícia Torquato Viana [2]; Heron Dominguez Torres da Silva [3]; Diogo Oliveira Silva [2]; Lucia Codognoto [4]

[1] Instituto de Ciências Ambientais, Químicas e Farmacêuticas / Universidade Federal de São Paulo - Campus Diadema; [2] Universidade Federal de São Paulo - Campus Diadema; [3] Departamento de Química / Instituto de Ciências Ambientais, Químicas e Farmacêuticas / Universidade Federal de São Paulo - Campus Diadema; [4] Universidade Federal de São Paulo - Campus de Diadema - SP

Chemical contaminants in the environment poses risks to public health.
Analytical procedures for removal of hormones in natural waters.
Destructive oxidation of hormones and full factorial design.

Environmental risk assessment of metals in contaminated sediments by industrial and port activities in Niterói, RJ

https://proceedings.science/p/120478

Rafaela Naegele [1]; Rodrigo Rocha [2]; Ricardo Soares [3]; Luís Clemens [4]; Maria Carla Santos [4]; Wilson Machado [5]; Ricardo Erthal Santelli [6]

[1] Diretoria de Pós-Licença / Instituto Estadual do Ambiente / INEA (Instituto Estadual do Ambiente); [2] INEA (Instituto Estadual do Ambiente); [3] INEA; [4] Universidade Federal Fluminense; [5] Departamento de Geoquímica / Instituto de Química / Universidade Federal Fluminense; [6] Departamento de Química Analítica / Instituto de Química / Universidade Federal do Rio de Janeiro

Cu and Zn concentrations were 110 to 202% above Conama Resolution 454 Level 2.
Zn presented a very high environmental risk due to concentrations in the exchangeable fractions (F1) of sediments.

Equilibrium studies of rare-earth elements biosorption by microbial cells

https://proceedings.science/p/120573

Ellen Cristine Giese [1]; Ana Carolina Sales Pereira de Souza [1]

[1] Centro de Tecnologia Mineral

Biosorption can be considered as a “green technology” solution for aqueous recovery environment. The biosorption capacity of La, Sm and Eu was investigated aiming lanthanide separation and recovery.

Estrogenic hormones removal in a wastewater treatment plant (WWTP) using membrane bioreactor (MBR)

https://proceedings.science/p/119637

Roberta Cerasi Urban [1]; Rafaela G. Machado [1]; Guilherme M. Grosseli [1]; Pedro Sergio Fadini [1]

[1] Universidade Federal de São Carlos

The presence of endocrine disruptors in the aquatic environment, especially natural and synthetic estrogens, has attracted the attention of researchers due to the impacts caused to organisms, such as damage to the reproductive system. In this context, the objective of the present study was to evaluate the occurrence, removal and space-temporal distribution of the estrogens at the Reuse Water Production Plant – RWPP Capivari II, (Campinas – SP) using a bioreactor coupled to membrane filtration (MBR). Samples collected monthly were filtered and the extraction of the analytes was performed using a solid phase extraction system. Estrogens were quantified using gas chromatography-mass spectrometry (GC-MS) and standard addition method. Estrogens concentrations (ng L-1) in the raw sewage ranged from 157.90 to 1,502.80 for estrone (E1), 46.44 to 1,419.78 for 17-β-estradiol (E2) and 83.56 to 132.52 for 17-α-ethinylestradiol (EE2). The removal rate of the target compounds was calculated considering their concentrations in the raw sewage and in the effluent of the MBR. Average removals of 72.5%, 33.7% and 28.7% were found for compounds E2, EE2 and E1 respectively. In relation to the behavior of estrogens throughout the sewage treatment, it was possible to observe an increase in the concentration of the compounds in some biological tanks. In general, a large part of the estrogens excreted by humans are originally present in conjugated forms (glucuronides and sulfates), however, they are deconjugated by microorganisms during biological treatment and this may explain the increase in the concentration observed in some tanks. Another point to be noted is the behavior of estrone at the end of biological treatment. According to Alvarino et al. (2014), the increase in estrone concentration may be a consequence of the partial oxidation of other estrogenic hormones to estrone.

Estudo da exposição ao mercúrio em lactantes da região Amazônica

https://proceedings.science/p/120192

Dayana Doffinger Ramos [1]; Reinaldo B. Possari Junior [2]; Rafael Piva Vasconcelos [3]; Pedro Magalhães Padilha [4]; Felipe Andre dos Santos [5]

[1] IFSP; [2] Engenharia de Biossistemas / FCE (Faculdade de Ciências e Engenharia) / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Programa de Pós Graduação em Química / Química / Universidade Federal de Mato Grosso do Sul; [4] Universidade Estadual Paulista "Júlio de Mesquita Filho" - Campus Botucatu; [5] Faculdade de Ciências e Engenharia - Unesp, Campus de Tupã

Study of mercury exposure in lactating women in the Amazon region. Mercury contamination in the Amazon region. Fish consumption leads to mercury contamination. Lactants contaminated with mercury.

Estudo da metilação do mercúrio no Pantanal Sul Mato-Grossense

https://proceedings.science/p/120225

Glaucia Almeida Nunes [1]; Dayana Doffinger Ramos [2]; Lincoln Carlos Silva de Oliveira [1]; Diovany Doffinger Ramos [3]; Ademir Santos [4]; Felipe Andre dos Santos [5]

[1] Instituto de Química da Universidade Federal de Mato Grosso do Sul; [2] IFSP; [3] Centro de Ciências Humanas e Sociais da Universidade Federal de Mato Grosso do Sul; [4] Instituto de Química - UNESP; Departamento de Química Analítica; [5] Faculdade de Ciências e Engenharia - Unesp, Campus de Tupã

Study of methylation of mercury in the Pantanal Sul Mato-Grossense. Gold mining presentes risk of contamination by methylmercury in the Pantanal. "Decoated" phenomenon enhances the methylation of Hg.

Estudo da utilização de fotocatalisadores na decomposição de petróleo em águas marinhas impactadas por derramamento

https://proceedings.science/p/120115

Stefanie Estrela Barbosa [1]; Marcos de Oliveira Melo [2]; Sarah Adriana Rocha Soares [3]

[1] UEFS; [2] Universidade Estadual de Feira de Santana; [3] UFBA

Study of the use of photocatalysts in the decomposition of oil in seawater impacted by spillage. Degradation of oil using two photocatalysts activated by sunlight. Spill simulation.

Estudo da viabilidade da casca de manga (Mangifera Indica) in natura como bioadsorvente em adsorção de chumbo em meio aquoso.

https://proceedings.science/p/119482

Rosemeire Santos [1]; Marcos Melo [1]; Klebson Souza Santos [1]; Taise Bonfim de Jesus [1]
[1] Universidade Estadual de Feira de Santana

Study of the viability of mango bark (Mangifera Indica) in nature, as an adsorbent for lead adsorption in aqueous media. Bioadsorption of Pb in water. Reutilization of mango fruit biomass.

Estudo de interação entre substâncias tipo húmicas extraídas de carvão hidrotérmico e íons Cu(II).

https://proceedings.science/p/120410

Bernardo Ribeiro de Moura [1]; Vinicius Sarracini Santos [2]; Marinônio Lopes Cornélio [2]; Stephane Mounier [3]; Marcia Bisinoti [4]; Altair Benedito Moreira [5]
[1] Instituto de Biociências, Letras e Ciências Exatas / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Institut Méditerranéen d'Océanologie; [4] Departamento de Química e Ciências Ambientais / IBILCE / UNESP (Universidade Estadual Paulista "Júlio de Mesquita Filho"- Campus São José do Rio Preto); [5] UNESP (Universidade Estadual Paulista "Júlio de Mesquita Filho"- Campus São José do Rio Preto)

O Brasil é o maior produtor de cana-de-açúcar do mundo, gerando elevadas quantidades de bagaço de cana-de-açúcar e vinhaça como subprodutos. A carbonização hidrotérmica possibilita a conversão dessas duas biomassas em um produto rico em matéria orgânica e nutrientes denominado carvão hidrotérmico (CH). O termo substâncias tipo húmicas (STH) refere-se aos extratos de diferentes materiais orgânicos que não foram submetidos ao processo natural de humificação no solo. As STH podem contribuir para o crescimento das plantas, aumentar a fertilidade biológica do solo e atuar na complexação de metais tóxicos. Este trabalho tem como objetivo estudar a interação de STH extraídas de CH com o metal Cu(II) empregando técnicas de supressão de fluorescência molecular, análise de correlação bidimensional de infravermelho (2D-COS-FTIR) e espectroscopia de fluorescência resolvida no tempo (TRFS).

Estudo do processo de destintagem enzimática de papel utilizando o fungo Aspergillus aculeatus

https://proceedings.science/p/120346

Ysabelli Maria Oliveira Catarino [1]; Enio Nazaré de Oliveira Junior [1]; Ana Maria de Oliveira [1]
[1] Universidade Federal de São João del-Rei

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Evaluation of the influence of humic substances on As(III) and As(V) toxicity by bioassays with Artemia salina

https://proceedings.science/p/120202

Aryanna Sany Pinto Nogueira Costa [1]; Amanda L. Alves Nascimento [1]; Cenira M. de Carvalho [2]; Josué Carinhanha Caldas Santos [3]; Daniela Santos Anunciação [1]
[1] UFAL; [2] Universidade Federal de Alagoas; [3] Universidade Federal de Alagoas

Natural and anthropogenic activities are increasing the concentration of arsenic (As) species in the environment so that, according to the Agency for Toxic Substances and Disease Registry (ATSDR), this element is at the top of the priority list of potentially toxic substances1 . Considering the evident interaction between As species and humic substances (HS) that can alter the characteristics of As species in the natural environment2 , this work aimed to evaluate the influence of humic substances (HS) on As(III) and As(V) toxicity to the microcrustacean Artemia salina. The experiments were performed in 10 mL test tubes containing 10 model organisms in the larval phase, under different concentrations of As(III) or As(V) standard solution (0.5 - 20 mg L-1), and fixed HS concentration (10 mg L-1). After times of 24, 48 and 72 h, the number of live larvae was checked by manual counting using a Pasteur pipette. For both As assays the control assay was performed. Afterwards, the effect of HS was evaluated, varying concentrations in 10, 20, and 40 mg L -1 , as well as the concentrations of As(III) standard solution, in a fixed time of 72 h. All experiments were performed in quadruplicate. According to the obtained results, the presence of HS in the Artemia salina cultures caused a reduction in the toxicity of the arsenic species to the microcrustacean, since the lethal concentration (LC50) was increased (Fig 1). For As(III), this difference was only verified significantly after 48 h of exposure, while for As(V)

there was a difference in the first 24 h. Finally, it was verified that the presence of HS promotes a positive effect to systems containing Artemia salina due to the reduction of the toxicity of the evaluated As species due to the As-HS complexation. Thus, it can be inferred that the interaction between humic substances and As(III) and As(V) present in aquatic environments, positively influences this type of environment.

EVALUATION OF ULTRAFILTRATION SYSTEMS FOR NATURAL WATERS IN AMAZON: SOLID PARTICLES, ORGANIC AND BIOLOGICAL CONTAMINATION

https://proceedings.science/p/119759

Nívea Cristina Guedes Munin [1]; Alex Ramos [2]; Kessia Sales [2]; Fábio Leonel [2]; Cassiana Carolina Montagner [3]
[1] UFAM/UNICAMP; [2] Universidade Federal do Amazonas; [3] Universidade Estadual de Campinas

The inorganic and organic coagulants used with ultrafiltration membrane were efficient in removing turbidity, suspended solids and organic compounds. The system can be used by "riverside communities".

Evaluation of UV radiation and oxidizing agents with multivariate analysis on the degradation of the 2,2-diphenyl-1-picrylhydrazyl residues

https://proceedings.science/p/120504

Kethlin Flora Curiel [1]; Wanessa Melchert Mattos [2]; Kethlin Flora Curiel [1]
[1] Escola Superior de Agricultura Luiz de Queiroz - Universidade de São Paulo; [2] Universidade de São Paulo

Total mineralization of the chemical residue (generated in the analysis of antioxidant activity - radical DPPH •) by advanced oxidative processes.

EXPLORATORY CHEMOMETRIC METHODS AS A MEANS OF INTEGRATED WATER QUALITY RESEARCH

https://proceedings.science/p/120637

Grazielle Rocha dos Santos [1]; Janine Trindade Pereira de Paula Batista [1]; Fernando Ítalo Miranda Góis [1]; Aníbal da Fonseca Santiago [1]; Gilmare Antônia da Silva [2]
[1] Universidade Federal de Ouro Preto; [2] Universidade Federal de Viçosa

Multivariate exploratory analysis techniques applied to environmental monitoring data. Water quality assessment of Doce river hydrographic sub-basin, Minas Gerais, Brazil.

FACTORIAL DESIGN APPLIED IN THE OPTIMIZATION OF ATRAZINE DEGRADATION APPLYING THE H2O2/UV-VIS HOMOGENEOUS PROCESS

https://proceedings.science/p/119798

Jennifer do Nascimento Chaves Menezes [1]; Murilo de Oliveira Souza [2]; Maria Cristina Canela [1]
[1] Universidade Estadual do Norte Fluminense Darcy Ribeiro; [2] Instituto Federal Fluminense

Advanced oxidative processes remove atrazine in water. Removal atrazine was optimized through a factorial design with two variables. The increase in temperature is a more significant factor for degrad

High Resolution Characterization of Sanitary Landfills Soil by Electrical Conductivity Probe

https://proceedings.science/p/119442

Osmar Francisco Gomes [1]

[1] CEPEMA - Poli - USP

The biggest challenge in investigating a contaminated area is accurate diagnosis. High Resolution Site Characterization (HRSC) of contaminated areas maps the subsurface every each 1.5 cm and it is being increasingly used and accepted in the field of soil contamination, for instance studies of environmental impact investigations. Soils with greater capacity to retain ions, such as clay and organic matrices, have higher electrical conductivity, mainly due to the presence of ions. When contaminated by landfill leachate, the studied soils undergo through several changes in concentration, resulting from the massive presence of larger ions as Ca2+, Mg2+ , Na+ , K+ , NH4 + , NO3 - , PO4 2- , Cl- , SO4 2- and HCO3 - , characteristics of percolates from this source.

Human health risk assessment of potentially toxic metals in spent fluorescent lamps

https://proceedings.science/p/119679

Camila Vicente de Farias [1]; Jéssica Frontino Paulino [2]; Daniel Alves Barcelos [3]; Ana Paula de Castro Rodrigues [1]; Fernanda Veronesi Marinho Pontes [2]

[1] Universidade Federal do Rio de Janeiro; [2] Departamento de Química Analítica / Universidade Federal do Rio de Janeiro; [3] Universidade de Lisboa

Human health risk assessment of Cd, Mn, Ni, and Zn in spent fluorescent lamps showed that Cd is a risk to children and adults. The results show the importance of the correct disposal of this waste.

In situ fluxes of labile metals at the soil/water interface of alkaline-saline lakes from Pantanal: A DGT-based approach

https://proceedings.science/p/120602

Jose Lucas Martins Viana [1]; Carlos Eduardo Eismann [2]; Lucas Pellegrini Elias [2]; Laurent Barbiero [3]; Amauri Menegário [2]; Anne Helene Fostier [1]

[1] Universidade Estadual de Campinas; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Institute of Research for Development

Fluxes of metals were determined at the soil/water interface of alkaline lakes of Pantanal. Only As, Fe, Mn and Zn were quantified. Fluxes of metals may be related to the water pH.

Investigation of ions sources in inhalabe particulate material in internal and external atmospheres in the North of Rio de Janeiro State.

https://proceedings.science/p/120001

Cibele Maria Stivanin de Almeida [1]; Vinícius Lionel Matheus [2]; Ana Fernandes Seares [1]

[1] Universidade Estadual do Norte Fluminense Darcy Ribeiro; [2] Universidade Federal do Espírito Santo, Brazil

The various ions sources were investigated for the first time
Relationships were established with the burning of sugar cane

It's raining emerging contaminants!

https://proceedings.science/p/119724

Mariana Amaral Dias [1]; Cassiana Carolina Montagner [1]

[1] Universidade Estadual de Campinas

Few studies about contaminants in rainwater are found in the literature. Emerging contaminants may be transported in the atmosphere for long distances.

Life Cycle Assessment of the Synthesis of Mixed Nano Structured Matrix Membranes with Metal Organic Frameworks

https://proceedings.science/p/119556

João Mario Brito Neto [1]; JUSSARA DE MIRANDA [1]

[1] Universidade Federal do Rio de Janeiro

Life cycle analysis (LCA) has been done as a method for assessing all direct and indirect environmental impacts of mixed matrix membranes (MMMs) with metal organic frameworks (MOFs). Mixed matrix membranes with MOFs and polymers (Figure 1) were previously synthesized and tested by our group. MMMs can be employed for different applications in the industry, such as: filters for water treatment, capture systems / permeability of gases such as CO2 and tests in the petrochemical industry. In addition to versatility in applications, MMMs prove to be advantageous from economic and energetic points of view. After the synthesis of MMMs with two MOFs- MIL-101(Cr) and MIL-53(Al), CO2 permeability was analyzed and compared to the MATRIMID 5218® membrane. Table 1 shows the higher CO2 permeability of the synthesized MMMs: MMM-10% (MIL-101(Cr) and MMM-10% (MIL-52(Al) in comparison with MATRIMID. as for the permeability of CO2, as demonstrated in table 1. LCA of both MMMsMMM10% (MIL-101(Cr) and MMM-10% (MIL-53(Al) as well as MATRIMID was done using UMBERTO NXT Software and the Ecoinvent v3® data platform. It was possible to model the processes of the three types of membranes studied and perform a comparison from the environmental point of view, that is, to assess the environmental impact that each of them generates from its productive process until the end of its "consumption". The 18 intermediate impact factors (or Midpoints) were determined with only 5 factors. The results showed that the most sustainable factors were Climate change (in kg CO2eq), Fossil depletion (in kg oil eq.), human toxicity (in kg 1,4-dcbeq.), metallic Depletion (in kg Fe eq.) and ionizing radiation (in kg U235 eq.).

Metal exposure biomarker evaluation in exposed atmospheric biomonitors in the port region of Niterói, RJ

https://proceedings.science/p/119851

Karmel Beringui [1]; Lucia Helena Sousa [1]; Tatiana Saint'Pierre [1]; Rachel Ann Hauser-Davis [2]; Adriana Gioda [1]

[1] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio); [2] Fiocruz

MT, GSH and total metal were determined in T. usneoides and T. stricta. Some metal elements may cause oxidative stress. Metal concentrations depend on the Tillandsia species.

Methylene Blue adsorption on Hydrochar obtained from sugarcane industry by-products

https://proceedings.science/p/120158

Márcio Justi Laranja [1]; Odair Pastor Ferreira [2]; Altair Benedito Moreira [3]; Marcia Bisinoti [4]

[1] IBILCE / UNESP (Universidade Estadual Paulista "Júlio de Mesquita Filho"- Campus São José do Rio Preto); [2] Universidade Federal do Ceará, Campus do Pici, Departamento de Física; [3] UNESP (Universidade Estadual Paulista "Júlio de Mesquita Filho"- Campus São José do Rio Preto); [4] Departamento de Química e Ciências Ambientais / IBILCE / UNESP (Universidade Estadual Paulista "Júlio de Mesquita Filho"- Campus São José do Rio Preto)

*The adsorption of methylene blue on hydrochar follows the kinetic model of pseudo-second order.
*Methylene blue is adsorbed on the monolayer, as predicted by the Langmüir model.

Murumuru Kernel Shell as Bioadsorbent for Dry Biodiesel Purification: Removal of Metallic Pollutants

https://proceedings.science/p/119920

Rafael Roberto Cardoso Bastos [1]; Victória Giovana do Nascimento Damasceno [1]; ANA PAULA DA CORREA [1]; Nathália Luiza Oliveira Costa [1]; Rafael Gonçalves Pontes [1]; Kelly das Graças Fernandes Dantas [1]; Leyvison Rafael Vieira da Conceição [1]

[1] UFPA

From all the contaminants of biodiesel, metals have received special attention due to the acceleration of biodiesel degradation processes. Aiming reduce the generation of wastewater or residual solvents, the present study objective to evaluate the use of murumuru kernel shell as a bioadsorbent for removal of contaminants Na, K, Ca, Mg, Cu and Fe

from crude soybean biodiesel – produced by homogeneous catalysis with KOH – and compare the results with conventional purification using deionized water. To obtain the bioadsorbent, murumuru kernel shell was crushed, sieved and kiln dried. The material was characterized by thermogravimetric analysis (TG) for determine the thermal profile and energy dispersion X-ray spectroscopy, for chemical composition (EDX). The crude biodiesel was separated from glycerol phase by decantation, and purified via wet (deionized water to 80 °C) and dry purified with murumuru adsorbent (3% w/v, at room temperature for 30 min). Determination of metallic contaminants before and after the purification processes was done by MIP-AES. The TG analysis revealed that the material remains stable at the employed temperature. The EDX analysis revealed SiO2 (37.2%) and CaO (33.1%) as major components, responsible for the high adsorptive capacity of metallic components (FOLETTO et al., 2020). ANP Resolution N° 45 (2014) establishes a maximum limit of 5 mg kg-1 for Na+K and Ca+Mg. For Ca and Mg, no significant levels were found in all investigated samples. For the other components, dry purification with murumuru bioadsorbent were better than purification with deionized water, since it was able to remove practically all contaminants investigated, while the water purification did not meet the limits established for Na and K. Thus, the use of murumuru kernel shell as bioadsorbent is an effective alternative for purification of crude biodiesel, enabling the reuse of this agro-industrial waste. FOLETTO, Edson Luiz et al. **Química Nova**, v. 28, n. 6, p.1055-1060, 2005.

Occurrence of 2,4-D and fipronil in mesocosm systems during the conventional management of sugarcane

https://proceedings.science/p/119728

Bianca Veloso Goulart [1]; Maria Paula Yoshii [2]; Isabele Baima Ferreira Freitas [3]; Erika Saldanha [4]; Luis Schiesari [2]; Evaldo Luiz Gaeta Espindola [3]; Cassiana Carolina Montagner [5]

[1] Universidade Estadual de Campinas - Instituto de Química; [2] Universidade de São Paulo; [3] Departamento de Hidráulica e Saneamento / Escola de Engenharia de São Carlos / Universidade de São Paulo; [4] Agência Paulista de Tecnologia dos Agronegócios (APTA); [5] Universidade Estadual de Campinas

This project evaluated the concentrations of fipronil and 2,4-D in mesocosm systems (9.000 L) during sugarcane management in a pasture conversion area in sugarcane fields. Monitoring of both pesticides was conducted in water samples from pasture, sugarcane crop and control areas, in a farm located in Brotas (São Paulo - Brazil), between 2018/Sep and 2020/Jan. The target pesticides were extracted using -solid phase extraction (SPE) with HLB Oasis 500 mg cartridges (Waters – Milford, USA). The quantification of the pesticides and their metabolites was performed on an Agilent 1200 Liquid Chromatography coupled to an Agilent 6410 triple quadrupole Mass Spectrometry with electrospray ionization (ESI). Initial sampling in Brotas indicated that the mesocosms presented trace concentrations of 2,4-D and fipronil, possibly due to residual application from the agricultural regions around the experimental farm. After pesticide application in sugarcane crop and intensive pasture areas, there was an increase of pesticide concentrations in the mesocosms -, which was not observed in the control mesocosm systems (unmodified pasture). In addition, an increase of concentration of fipronil after application of vinasse was observed during the management of year cane (cane stalks resprouting). The average concentrations of 2,4-D and fipronil after first and second applications (1400 and 41795 ng L-1 for 2,4-D and 37 and 47 ng L-1 for fipronil) were higher than water quality criteria (WQC) (200 e 12 ng L-1, respectively) indicating potential risk to aquatic life. However, the residual concentrations of pesticides in the sugarcane crop and intensive pasture areas were similar to those observed in the control mesocosms even months after their application in the first cycle management.

Occurrence of disinfection by-products in wastewater treatment plants – a look at the potable reuse viability

https://proceedings.science/p/119757

Raphael Acayaba

More than 600 DBPs are identified and cataloged, but little is known about their occurrence in the environment and the real impact on human health.

Optimization of a low volume extraction method to determine polycyclic aromatic hydrocarbons (PAH) in aerosol samples

https://proceedings.science/p/119804

Caroline Scaramboni [1]; Jordan Brizi Neris [2]; Edenir Rodrigues Pereira Filho [2]; Roberta Cerasi Urban [2]; Maria Lúcia Arruda de Moura Campos [3]

[1] Departamento de Química / Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto / Universidade de São Paulo; [2] Universidade Federal de São Carlos; [3] Universidade de São Paulo

Extraction conditions were optimized using design of experiments, and provided a method with reduced solvent volume to determine polycyclic aromatic hydrocarbons and derivatives in aerosol samples.

Optimization of analytical method to quantify pesticides in soil

https://proceedings.science/p/119779

Ingrid Ruanna dos Santos Feitosa [1]; Bianca Veloso Goulart [2]; Cassiana Carolina Montagner [1]

[1] UNICAMP; [2] Universidade Estadual de Campinas - Instituto de Química

Optimization of solid-liquid extraction for determination of 7 pesticides in soil samples. Recoveries between 90 – 119 % were obtained using the best conditions.

Oxidation degree of microplastic collected from surface freshwater in the Guaíba Lake, Porto Alegre x0096 Brazil

https://proceedings.science/p/119476

Crislaine Bertoldi [1]; Larissa Zacher Lara [1]; Fernanda Martins [1]; Andreia Neves Fernandes [1]

[1] Universidade Federal do Rio Grande do Sul

187 items were identified as polymer in the surface freshwater samples from Guaíba Lake.
58% of microplastics were highly oxidized related to a long residence of these particles in the aquatic lake

Perfil epidemiológico de vítimas de intoxicação por Aldicarbe no Estado da Bahia no período de 2012 a 2015

https://proceedings.science/p/120397

Lícia Passos dos Santos Cruz [1]; Winne Figueiredo Ribeiro [1]; Luiz Marcos Vita Machado [2]

[1] Universidade Federal da Bahia; [2] Departamento de Polícia Técnica da Bahia

Descriptive analysis of the mortality profile by Aldicarb poisoning in the Bahia from 2012-2015 was made, showing that even with reduction of fatal intoxications, this remains problem of public health

Pesticides behavior in the atmosphere of an urban area in Brazil. Risk assessment for human health.

https://proceedings.science/p/120146

Aleinnys Marys Barredo Yera [1]; Pérola de Castro Vasconcellos [1]; Sofia Caumo [1]

[1] Universidade de São Paulo

In the last few years, different types of pesticides have been detected in the atmosphere in rural and urban areas around the world. These, are chemical compounds used in agriculture to avoid plague, rodents, fungi and unwanted plants. Besides that, they are often used in public health to kill vectors of disease,such as mosquitoes. Some studies have showed the relations between pesticides exposure and some diseases, such as autoimmune and cardiovascular diseases, and respiratory problems. An attempt to investigate the composition of PM in the neighbor atmosphere of an industrial complex has been proposed in the last years due to the high rate of thyroid diseases in the population living near this region. In this work was determined the concentrations of pesticides in samples collected between 2015, 2016 and 2017 at an industrial and urban area. The assessment of the risk caused by inhalation of these compounds

was calculated. Samples (n=42) were extracted and 11 pesticides were determined by gas chromatography coupled to a mass spectrometer. Samples collected in 2017 showed the higher concentrations. Pesticides such as malathion and permethrin, used in the control of domestic pests, presented the highest concentrations (537 pg m-3and 625 pg m-3 respectively) due to the wide use in this area. The highest values of daily inhalation exposure were for heptachlor in infants, 2 x 10-4mg kg-1 day-1. All values of the hazard quotients are lower than 1indicating that there is no danger to human health by inhalation. Cancer risk was found for heptachlor in adults, infants and children in the three years.

Highlights

- First determination of pesticides in the atmosphere of Capuava.
- All measured reported Hazard Quotients <1.
- Cancer risk was found for heptachlor in adults, infants, and children.

Photodegradation of 2,4-dichlorophenoxyacetic acid using chitosan-based polymer membranes containing encapsulated metal oxides

https://proceedings.science/p/120635

Mauricio Paz [1]; Tifani Ferens [1]; Natália Lang [1]; Heveline Enzweiler [1]; Alexandre Tadeu Paulino [1]; Mauricio Paz [1]; Tifani Franco Ferens [1]; Natália Soccio Lang [1]

[1] Universidade do Estado de Santa Catarina - UDESC

- Chitosan-based membranes containing metal oxides were synthesized - Photodegradation of 2,4-dichlorophenoxyacetic acid in water - Purification of water and wastewater by photocatalytic degradation

Pollutants and biomarkers in Piaractus mesopotamicus (Pacu) and Semaprochilodus sp. (Jaraqui) marketed in Manaus, Amazonas, Brazil

https://proceedings.science/p/120287

Tereza Cristina Souza de Oliveira; Milton Costa Viana [1]; Bárbara Sarmento [1]; Taynara Soares Vale [1]; Larissa Torrezani [2]; Nilda Gorete Palma Pantoja [3]; Letícia A. Sbrocca [4]; Rodrigo Pedrosa [4]; Lucia Helena Sousa [5]; Rachel Ann Hauser-Davis [6]; Adriana Haddad Nudi [7]

[1] UFAM; [2] SGB/CPRM; [3] CPRM; [4] FIOCRUZ; [5] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio); [6] FIOCRUA; [7] PUC-Rio

Samples from two fish species, Piaractus mesopotamicus (Pacú) and Semaprochilodus sp. (Jaraqui), sold at an open market in Manaus, Amazonas, Brazil were analyzed concerning metal and oxidative stress biomarkers in muscle tissue. Chromium (Cr), Copper (Cu), Cadmium (Cd), Zinc (Zn), were analyzed after soft extraction by Inductively Coupled Plasma Mass Spectrometry (ICP-MS, Limit of quantification (LQ) 0.01 – 0.075 mg kg-1), Total mercury (Hg) was analyzed by Direct Mercury Analysis System DMA-80 (LQ = 0.0005 mg kg-1), while metallothionein (MT) and Reduced glutathione (GSH) were assessed by UV-Vis spectrophotometry. Preliminary results indicate public health concerns regarding the consumption of these fish, as both Jaraqui and Pacú muscle tissues presented Cr above the respective maximum permissible ingestion limit as stipulated by the Brazilian ANVISA (Figure 1). It seems that both species display the same level of MT induction, while 2.4-fold higher GSH levels were noted in Jaraqui. In addition, higher metal concentrations were observed in this species, except for Cd, and Hg was up to 3.9-fold higher compared to Pacú, probably due to the fact that this is a detritivorous species, while Pacú are omnivorous. Further assessments will be carried out with 40 individuals purchased in Manaus markets originating from the Purus River, according to fish sellers, and statistical correlations with the oxidative stress biomarkers shall be carried out.

Production and characterization of aromatic biolubricants from soybean oil

https://proceedings.science/p/120401

Ana Luiza Reis Rodrigues da Cunha [1]; Lilian Ribeiro Batista [1]; Aline Silva Muniz [1]; Nelson Roberto Antoniosi Filho [1]

[1] Universidade Federal de Goiás

Chemical modification of soybean oil by transesterification reaction and the addition of aromatic molecules to unsaturation. Physical-chemical characterization for application as biolubricants.

Remoção de ácido salicílico em águas por adsorção em carvão ativado obtido da casca do coco licuri

https://proceedings.science/p/120247

Larissa Silva de Oliveira Mota [1]; Bruno Salarini Peixoto [2]; Marcia Cristina da Cunha Veloso [1]; Gilberto Alves Romeiro [1]; Marcela de Moraes [1]

[1] UFF; [2] Universidade Federal Fluminense

The KOH activation resulted in a material with 3 times the adsorption capacity of the commercial activated carbon.

Remoção de bisfenol-A por bioadsorventes produzidos a partir de serapilheira coletada na Baía de Todos os Santos

https://proceedings.science/p/120090

Matheus Chaves Moreira da Silva [1]; José Luiz Cunha Cordeiro [1]; Artur José Santos Mascarenhas [2]; Raildo Alves Fiuza Junior [1]

[1] Universidade Federal da Bahia; [2] Univeridade Federal da Bahia

Bisphenol-A removal by bioadsorbents produced from plant litter collected in Todos os Santos Bay The precursor used for the production of activated carbon is promising Materials activated with H3PO.

Remoção fotocatalítica de dimetil sulfeto utilizando compósitos de argila-TiO2

https://proceedings.science/p/120451

Juliana Carvalho [1]; Maria Cristina Canela [2]; Benigno Sanchez [3]

[1] Universidade Estadual do Norte Fluminense (UENF) e Universidade Federal Fluminense (INFES-UFF) ; [2] Universidade Estadual do Norte Fluminense Darcy Ribeiro; [3] CIEMAT

Brazilian clay-TiO2 composites for photocatalytic removal of dimethyl sulfide The use of hybrid clay-TiO2 photocatalysts as an adsorbent was evaluated for photocatalytic degradation.

Removal efficiency and seasonal variation of pharmaceuticals in drinking water treatment plants

https://proceedings.science/p/119611

Lucilaine Valéria de Souza Santos [1]; Eduarda Oliveira Reis [2]; Victor Rezende Moreira [2]; Yuri Abner Rocha Lebron [2]; Míriam Cristina Santos Amaral [2]; Liséte Celina Lange [2]

[1] Pontifícia Universidade Católica de Minas Gerais (PUC Minas); [2] Departamento de Engenharia Sanitária e Ambiental (DESA/UFMG)

The presence of pharmaceuticals in environmental waters has become a major issue and concern for the scientific community. In Brazil several cities don't have wastewater treatment plants and sewage is often disposed directly into the rivers. This sanitation condition affects the water quality in the rivers and drinking water production, since Drinking Water Treatment Plants (DWTPs) mainly draw water from these sources. The behavior of pharmaceuticals in full-scale conventional DWTPs remains less-known, especially in Brazil. Thus, the objective of this study was to investigate if there is a seasonal variation on the removal efficiency (RE) of the pharmaceuticals Prednisone (PRE), Atorvastatin (ATO) and Fluconazole (FLU) in three Brazilian conventional DWTPs. Samples were collected for twelve months (ago/16 to jul/17) in three DWTPs of Minas Gerais state. The analytical methodology was based on solid phase extraction (C18 cartridge) followed by High-Performance Liquid Chromatography (Prominence DGU/20A3 – Shimadzu) coupled with Mass Spectrometry (MicroTOF-QII –Bruker). The monitoring results showed the presence of the pharmaceuticals FLU (107 – 1413 ng/L), PRE (56 – 2632 ng/L) and ATO (109 – 639 ng/L) in both source and drinking water. The RE varied between the pharmaceutical compound and DWTP. Besides, it was observed the greater temporal variation of RE in the different DWTPs. This seasonal variation of the RE in conventional DWTPs was also reported by others authors, suggesting that the source water quality may impact the RE of the DWTPs and that conventional DWTP are inefficient in completely removing pharmaceutical compounds

REMOVAL OF ACETAMINOPHEN BY LACCASE IMMOBILIZED IN AVOCADO SEED BIOCHAR

https://proceedings.science/p/119620

Chrys Katielli Hoinacki da Silva [1]; Pedro M. Cabrera [1]; Pascal S. Thue [1]; Éder C. Lima [1]; Roberta Bussamara [1]; Andreia Neves Fernandes [1]

[1] Universidade Federal do Rio Grande do Sul

Laccase-based bioprocesses represent a fascinating perspective for the removal of emerging contaminants in waters and wastewaters. Biocatalytic treatment using oxidoreductase enzymes, especially laccases, has received the attention of the scientific community for biodegradation of pharmaceutical compounds, such as acetaminophen, to less harmful compounds. However, enzymes are required to be immobilized on supports to be reusable and maintain their activity. In this study, the laccase from Trametes versicolor was immobilized in avocado seed biochar to remove acetaminophen (ACT) from aqueous solution. Initially, the preparation of the avocado seed biochar (ASB) was carried by pyrolysis of avocado seed at 500°C for 30 min. Afterward, two treatments were employed to activate the pyrolyzed material. In the first treatment, 2 g of ASB material was treated with 50 mL of 2 mol L−1 citric acid by shaking at 80 rpm for 24 h. The activated biochar was labeled as A-ASB. In the second treatment, 50 mg of treated material with citric acid was placed in contact with 10 mL of glutaraldehyde 1% and 5% (v/v) for 3 h at 80 rpm. These samples were labeled as G1A-ASB and G5A-ASB, respectively. The immobilization procedure was performed by mixing 10 mg of samples ASB, A-ASB, G1A-ASB, or G5A-ASB with 7.5 U of laccase enzyme (U = enzyme unit) in pH 5.0 at 25°C under agitation at 50 rpm for 24h. After immobilization, enzymatic activity was determined by oxidation of 2,2-azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) to cationic radical ABTS+, which was quantified by UV-Vis spectroscopy (ʎ = 420 nm). The results shown in Figure 1 demonstrate that the material G1A-ASB presented higher immobilization efficiency (IE) and a higher activity of laccase (U) by gram of material (U/g). Therefore, G1A-ASB support with immobilized laccase was applied in the removal of ACT. For this, 10 mg of support with and without immobilized laccase was placed in contact with 5 mL of ACT (30 mg L-1) for 24 h at 80 rpm. After, ACT concentration in the supernatant was measured by capillary electrophoresis. The results (Figure 2) show that the support without laccase (G1A-ASB) removed only 7% of ACT, while the support with immobilized laccase (LG1A-ASB) removed 73%. Thus, this study demonstrated that avocado seed biochar has potential to be used as support in laccase immobilization since the laccase remained active in support, degrading the ACT.

Removal of phosphate from waters with Fe(III)-polyhydroxy cations supported onto montmorillonite K10 (MT)

https://proceedings.science/p/120193

Samara Leite [1]; Jorge Masini [1]; Fernando Nascimento [1]

[1] Instituto de Química da USP

The commercial K10 montmorillonite was modified with Fe3+ polyhydroxy cations aiming at the enhancement of adsorption affinity towards phosphate anions, which are known to cause eutrophication in lakes and reservoirs. Polyhydroxy cations with OH-: Fe3+ molar ratios of 0.75:1, 1:1 and 2:1 were investigated. The incorporation of the polycations did not alter the main conformational characteristics of the montmorillonite, as verified by surface area measurements, X-ray diffractometry, FTIR, electron microscopy and zeta potential titrations. On the other hand, the materials supporting Fe3+ polyhydroxy cations exhibited a significant enhancement of adsorption capacity (qmax), as determined by Langmuir isotherms, from 1.7 ± 0.1 to 2.8 ± 0.1 μmol g-1, and the adsorption energy from 0.062 to 0.26 L mg-1. The different ratios of OH- to Fe3+ did not affect the adsorption capacities. The adsorption kinetics was best described by the pseudo 2nd order model, with the equilibrium being approached within 120 min of contact time. The adsorption was independent of pH in a pH range between 4.6 and 8.5. The increase in ionic strength increased the adsorption capacities indicating that the formation of inner-sphere complexes prevail over electrostatic interactions in the adsorption mechanism. The materials were tested for removing phosphate from three polluted water samples with phosphate concentrations between 0.0919 and 1.211 mg L-1. The removal was quantitative and the remaining phosphate was below the limit of detection of the analytical method. The presence of 10 mg L-1 humic or fulvic acid did not affect the performance of the materials. Thus, we believe that the modification of clay minerals with Fe3+ polyhydroxy cations is suitable to produce low-cost adsorbents for phosphate.

Risk is in the air: Oxidative Potential of Atmospheric Particulate Matter Collected near an Industrial Complex in São Paulo.

https://proceedings.science/p/119687

Pérola de Castro Vasconcellos [1]; Sofia Caumo [1]; Alisson Traub [2]; Greg Evans [2]
[1] Universidade de São Paulo; [2] University of Toronto

-Air particulate matter collected between 2015 and 2018 near an industrial complex showed high antioxidant depletion capacity. -The oxidative potential activity is linked to hospital admissions.

Síntese e uso de material híbrido metal-orgânico UiO-66 (Zr) para captura de gases do efeito estufa e transporte de fármacos

https://proceedings.science/p/120236

Hiasmin Christine Kurrle Pinheiro Sodre [1]; Jussara Lopes de Miranda [2]; João Mario Brito Neto [3]; Stevan Matheus Maranha dos Santos [3]; Guilherme Sales [3]
[1] INSTITUTO DE QUIMICA- UFRJ; [2] INSTITUTO DE QUÍMICA - UFRJ; [3] Universidade Federal do Rio de Janeiro

- Synthesis, characterization of metal organic framework UIO-66 in a sustainable way
- Adsorption of greenhouse gases and study of drug delivery using MOFs

Size distribution of mass and chemical composition of particulate matter in metropolitan area of São Paulo in winter (2017-2018)

https://proceedings.science/p/120010

Adalgiza Fornaro [1]
[1] Universidade de São Paulo

Solid supports covered by bixin as a selective gold biosorbent from aqueous systems

https://proceedings.science/p/120473

Mariana Cristine Coelho Diniz [1]; Júlia Condé Vieira [1]; Ricardo Mathias Orlando [1]; Guilherme Dias Rodrigues [1]; Rubén Sinisterra [1]
[1] Universidade Federal de Minas Gerais

Bixin was incorporated on different supports by deep coating
Bixin was selective for Au in the presence of Fe(III) and Mn(II)
A maximum recovery of 80 ± 2 % was obtained without any prior optimization

Sorption characteristics of endocrine disrupting compounds (EDC) on polyamide microplastics

https://proceedings.science/p/119595

Larissa Zacher Lara [1]; Crislaine Bertoldi [1]; Nortom Munhoz Alves [1]; Fernanda Martins [1]; Andreia Neves Fernandes [1]
[1] Universidade Federal do Rio Grande do Sul

Microplastics are small plastic debris that threat environment biota
Interactions between EDC and polyamide microplastics were investigated
Microplastics sorbed up to 80% of EDC in aqueous solution

Study of partitioning of hormones from water samples using aqueous two-phase systems.

https://proceedings.science/p/120756

Junielly Tomaz Domingues [1]; Aparecida Barbosa Mageste [2]; Leandro Rodrigues de Lemos [3]; Ricardo Mathias Orlando [1]; Guilherme Dias Rodrigues [1]

[1] Universidade Federal de Minas Gerais; [2] Universidade Federal de Ouro Preto; [3] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Aqueous two-phase system was applied as an environmentally friendly liquid-liquid extraction technique.
The optimized systems were able to partition efficiently (K > 38) five steroid hormones.

Synthesis of polymeric microparticles for application as agricultural fertilizer utilizing multivariate optimization methods

https://proceedings.science/p/120639

Júnior Olair Chagas [1]; Monteiro Carlos Monteiro Mapero [2]; Célia Machado Ronconi [1]; Gilmare Antônia da Silva [3]; Fabiana Aparecida Lobo [4]

[1] Universidade Federal Fluminense; [2] Programa de Pós-Graduação em Química / Departamento de Química / Universidade Federal de Ouro Preto; [3] Universidade Federal de Viçosa; [4] Universidade Federal de Ouro Preto

Multivariate optimization used to obtain the best synthesis conditions of polymeric microparticles.
Modified release system of metallic cations as an alternative fertilizer for agricultural.

Treatment of antibiotic amoxicillin in water by UV/H2O2

https://proceedings.science/p/120113

Gabriela Vettorello [1]

[1] UNIVATES

Utilização de biomassa de casca de aipim (Manihot esculenta) in natura como bioadsorvente de Cd e Pb meio aquoso.

https://proceedings.science/p/119499

Ana Caroline Amorim de Oliveira [1]; Marcos de Oliveira Melo [1]; Isabela Garcia Marinho [1]

[1] Universidade Estadual de Feira de Santana

Utilização de uma argila natural para a remoção do corante azul de metileno em meio aquoso

https://proceedings.science/p/119671

Jose Milton de Matos

Utilização do planejamento experimental na escolha de condições ótimas de adsorção de Cd e Pb em biomassa de acerola (Malpighia punicifolia L.).

https://proceedings.science/p/119538

Isabela Garcia Marinho [1]; Marcos Melo [1]; Klebson Santos [1]

[1] Universidade Estadual de Feira de Santana

Use of experimental planning in the choice of optimal conditions for adsorption of Cd and Pb in acerola (Malpighia punicifolia L.) biomass. Factorial planning.Bioadsorption Cd,Pb. Acerola seed biomass

UV radiation, High Power Ultrasound and 70% hydrogen peroxide in the treatment of craft beer wastewater

https://proceedings.science/p/119838

Elisson Andrade de Souza [1]; Luciana Almeida da Silva [1]
[1] Universidade Federal da Bahia

* Craft beer wastewater treatment by Fenton, photo-Fenton and sono-Fenton processes. * Photo-Fenton process promotes 84% mineralization of absorbent species.

Química Analítica - ANA

Estudos para determinação simples e rápida de minoxidil em cosméticos falsos e urina usando eletrodo de diamante dopado com boro com voltametria de onda quadrada

https://proceedings.science/p/120765

Anne Alves Macedo [1]; Dilton Martins Pimentel [1]; Wallans Torres Pio Santos [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

This work presents a simple and fast electrochemical detection of minoxidil in fake cosmetic and urine samples using unmodified electrode with square wave voltammetry

A different approach for electromembrane extraction of naphthenic acids from aqueous sample followed by high-resolution mass spectrometry analysis

https://proceedings.science/p/120758

Giovanna Lopes de Araújo [1]; Rafael Oliveira Martins [1]; Marcella Ferreira Rodrigues [1]; Rosy Simas [2]; Andréa Rodrigues Chaves [1]; Boniek Gontijo Vaz [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal do Rio de Janeiro

This work demonstrates a modification of the conventional electromembrane extraction technique for the analysis of naphthenic acids using high-resolution mass spectrometry.

A Green Sample Preparation Method for further Determination of Elemental Impurities in Oily Pharmaceutical Excipients by ICP-OES

https://proceedings.science/p/119701

Cristian Andriolli [1]; Mariele Samuel do Nascimento [1]; Daniele Bandeira Silva [1]; Eder Flores [2]; Rochele Picoloto [1]; Erico Marlon de Moraes Flores [1]
[1] Universidade Federal de Santa Maria; [2] Universidade Tecnológica Federal do Paraná

The RP-DLLME method allowed the use of a high sample mass.
Low detection limits were obtained by ICP-OES.
The simultaneous extraction of As, Cd, Hg, Pb, Co, Ni, and V was performed.

A NEW ELECTROCHEMICAL SENSOR BASED ON OXIDIZED CAPSAICINA+MWCNT ON GLASSY CARBON ELECTRODE FOR URIC ACID QUANTIFICATION

https://proceedings.science/p/120022

Dave Di Everton Rufino dos Santos [1]; Andresa Katherinne Albuquerque de Almeida [1]; Marília Oliveira Fonseca Goulart [1]; Leonardo Vieira da Silva [2]; Nicholas Deymisson dos Santos [1]

[1] Universidade Federal de Alagoas; [2] Instituto Federal de Alagoas

Electrochemical sensors are devices capable of collecting data with minimal manipulation of the system, with some drawbacks like surface poisoning and high over voltages to oxidize (or reduce) the analytes. It is possible to immobilize chemical species on the electrode surface in order to increase its sensitivity and selectivity in the detection of molecules of biological importance, such as Uric Acid (UA). UA is a biomolecule produced by the catabolism of purines that when found in high concentrations in the body indicates the clinical disorder known as Gota. A system of three electrodes in a glass cell (5 mL) was used: chemically modified Glassy Carbon Electrode (GCE), auxiliary electrode (platinum wire) and reference electrode (Ag/AgCl). Capsaicin was polymerized on GCE/MWCNT being important as redox mediator for electroanalysis of uric acid in blood plasma.

A UPLC®–MS/MS targeted plasma metabolomics on neuropathic pain rats

https://proceedings.science/p/119855

Lucas Maciel Mauriz Marques [1]; José Carlos Tomaz [2]

[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP); [2] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP)

Identification and quantification of neuropathic pain biomarkers. Targeted metabolomic method development and validation

Alternative sorbent for SBSE and the application for extraction of triazines

https://proceedings.science/p/120561

Sara Renata Gonçalves [1]; Luis Fernando Amorim Batista [1]; Duanne Maciel Scremin [1]; Natascha Amalio Teixeira [1]; Sônia Faria Zawadzki [1]; Gilberto Abate [1]

[1] Universidade Federal do Paraná

Stir-bars were produced using a polyurethane elastomer and montmorillonite. The bars were investigated to extract triazines from aqueous medium. Sorption results demonstrated satisfactory results.

Analysis of St. Johnx0092s Wort by Paper Spray Mass Spectrometry

https://proceedings.science/p/119750

Ana Gabriella Carvalho Miguita [1]; Clésia Cristina Nascentes [1]; Marcelo Martins de Sena [1]

[1] Universidade Federal de Minas Gerais

Among the 30 analyzed samples of Hypericum perforatum L., 65.5% contained ions referring to another active ingredient.

Aplicações de métodos de preparo de amostras ambientais e alimentos

https://proceedings.science/p/120699

Jeancarlo Pereira dos Anjos [1]

[1] Centro Universitário SENAI CIMATEC

São apresentadas aplicações de técnicas de preparo de amostras para a determinação de analitos em matrizes ambientais e alimentos. Métodos como microextração com gota única (SDME), extração por Soxhlet, extração pelo método de Bligh & Dyer e extração com fluído supercrítico (SPE) foram aplicados na determinação de analitos de diferentes classes químicas em amostras como água de coco, vinhos, água superficial e subterrânea, além da extração

de óleo de sementes de uvas. Também, tem-se a aplicação de métodos de derivatização, para a determinação de compostos carbonílicos livres e ligados, em amostras de material particulado atmosférico (PM10), bem como a análise direta de mercúrio em amostras de material particulado atmosférico (PM2,5 e PM10) e combustíveis.

Application of mixture design using diluted acid for ultrasound-assisted extraction for determination trace elements in particulate matter by ICP-MS

https://proceedings.science/p/120456

Melina do Espírito Santo Lemos [1]; Carolina Scocco Provete [1]; Bruna Dalfior [1]; Vinicius Câmara Costa [1]; Geisamanda Pedrini Brandão [1]; Maria Tereza Carneiro [2]
[1] Universidade Federal do Espírito Santo; [2] UFES

Trace elements in particulate matter. Optimization of ultrasound-assisted extraction. Chemometric analysis.

Automated and simultaneous analysis using electronic eye associated with machine learning for wide beer quality control

https://proceedings.science/p/120067

João Victor de Sousa Dutra [1]; Ricardo Cunha Michel [1]; Daniella Lopez Vale [1]; Maiara Oliveira Salles [1]
[1] UFRJ

Using electronic eye to analyze beer is a common type of characterizing styles by hue in brewery's laboratories, but using only one parameter is not enough to consistently identify the various types of this beverage. Another barrier is to put the optical analysis inside the brewing process, avoiding this laboratory analyses. This study aims to overcome this barriers by creating and electronic eye which can analyze the hopped wort, the brewing wort and the beer at real time, doing the quality control. In this initial phase, the electronic eye was designed, programmed and built from scratch, with cheap elements; then twenty three beers, in a wide range of styles and labels, were analyze by this device, getting the frontal and lateral HSV color space of each sample, storing the data in a database. Then, an artificial neural network (ANN) code was wrote to classify the data and make predictions of style and label, by only using the beer's image. The six parameters were weighted and, by this point, the frontal hue and both frontal and lateral values were rated, by the deep machine learning code, the most important parameters of this analysis. This process had very precise and accurate responses using validation tests in about twenty five seconds, from getting the beer image, comparing it to the database and the program giving an accurate answer. Although the project seems promising, there is much more to optimize and improve, to make faster and more accurate analyses. This study can be considered a first application of this combined process inside the brewing process, that can be faster, more accurate and cheaper.

Avaliação da regressão linear As/V como ferramenta para diagnóstico de transporte de sedimento nas praias do Espírito Santo

https://proceedings.science/p/120511

Matheus Barbosa Rasch [1]; Maria Tereza Carneiro [2]; Jefferson Souza [1]; Bernardo Gasperazzo Urquia [1]; Bruna Correa [1]; Vinicius Câmara Costa [1]; Maiara Krause [1]; Geisamanda Pedrini Brandão [1]; Jacqueline Albino [1]
[1] Universidade Federal do Espírito Santo; [2] UFES

Evaluation of As/V linear regression as a tool for the diagnosis of sediment transport on the beaches of Espírito Santo. Determination of As and V. Diagnosis tool. Cross-shore sediment transport.

Avaliação do método de extração por banho ultrassônico na determinação de Li, Na e K na polpa de caju por fotometria de chama

https://proceedings.science/p/119627

Rosivaldo Sousa [1]; Francisco Panero [1]; Mirla Janaina Augusta Cidade [1]
[1] Universidade Federal de Roraima

Bioimaging of La in rat kidney by LA-ICP-MS following treatment with La2O3-NPs

https://proceedings.science/p/120419

Graciela Marini Heidrich [1]; Vinicius Machado Neves [1]; Ana Caroline Vedovato Rubin [1]; Agnes Souza Vaz [1]; Valderi Luiz Dressler [1]

[1] Universidade Federal de Santa Maria

Evaluation of biodistribution of La in biological sample, to understand the nanotoxicity of La2O3-NPs.
The LA-ICP-MS was used for the evaluation of La distribution.

Caracterização de Amostras de Óleo Provenientes do Derrame de Petróleo na Costa Litorânea de Pernambuco por GC-MS/MS

https://proceedings.science/p/119919

Ignes Regina dos Santos [1]; Rayane Nascimento [2]; Jhonattas Carregosa [3]; Alberto Wisniewski Jr [4]; Alex Souza Moraes [5]; Jandyson Machado Santos [5]

[1] UFRPE/PROGRAMA DE PÓS-GRADUAÇÃO EM QUIMICA; [2] Universidade Federal Rural de Pernambuco (UFRPE)/ Programa de Iniciação Científica, Departamento de Química.; [3] Universidade Federal de Sergipe (UFS)/ Centro de Ciências Exatas e Tecnologia; [4] Universidade Federal de Sergipe, Brasil.; [5] Universidade Federal Rural de Pernambuco (UFRPE)/ Programa de Pós-Graduação em Química, Departamento de Química.

- Biomarkers of oil spill samples identified by GC-MS/MS;
- Evidences of distinct chemical composition among the samples but no conclusive results;
- Need for advanced techniques such as FT-MS.

Caracterização do Insumo Farmacêutico Ativo Sulfato de Atazanavir

https://proceedings.science/p/120303

Emiliana Moraes de Carvalho [1]; Erika M. de Carvalho [1]; July A. H.Muñoz [1]

[1] Fiocruz

Desenvolvido e comercializado pelo laboratório Bristol Myers Squibb (BMS), o Sulfato de Atazanavir, de nome comercial Reyataz, é um antirretroviral (ARV) de segunda geração pertencente à classe dos inibidores de protease. Indicado em combinação com outros agentes antirretrovirais para o tratamento da infecção por HIV-1, faz parte do coquetel distribuído gratuitamente pelo Departamento de DST, Aids e Hepatites Virais, do Ministério da Saúde. A ANVISA, membro permanente do ICH desde 2016, tem agora a obrigatoriedade de se adequar às normas internacionais de qualidade para registro de medicamentos. Neste contexto, o controle de qualidade do produto acabado é de extrema importância, uma vez que é requerido o estabelecimento de limites seguros de impurezas para garantir a qualidade do medicamento. Definidas como sendo qualquer composto químico presente na formulação que não seja o Insumo Farmacêutico Ativo (IFA) ou os excipientes, essas presenças indesejáveis podem influenciar na segurança e eficácia do medicamento, por isso devem ser controladas desde os estágios iniciais de desenvolvimento de um produto. Nos compêndios oficiais, cujo objetivo é auxiliar na promoção da saúde da população, por meio do estabelecimento de requisitos de qualidade e segurança para fármacos, o método para controle de qualidade do IFA e produto acabado do Sulfato de Atazanavir só é encontrado na WHO, no entanto, nenhuma impureza conhecida é apresentada. Na literatura, artigos demonstram o desenvolvimento de métodos para quantificação do ativo e suas impurezas de degradação por técnicas cromatográficas, mas pouca informação é encontrada sobre caracterização do ativo e de suas impurezas. Sendo assim, o objetivo deste trabalho é apresentar a caracterização do IFA por meio dos métodos térmicos (DSC e TGA), espectroscópicos (RMN, IV e DRX) e cromatográficos, para auxiliar na elucidação estrutural de seus produtos de degradação. Foi utilizada cromatografia líquida de alta eficiência (CLAE) para desenvolvimento do método indicativo de estabilidade para determinação de Teor e Impurezas, seguindo RDC nº166, legislação brasileira vigente sobre validação analítica. Ainda em atendimento a legislação, adotou-se como referência a RDC nº53 para realização de testes iniciais de degradação forçada com o IFA, com o intuito de identificar das condições mais susceptíveis à degradação e onde ocorre maior formação de impurezas. Os testes de caracterização do IFA já foram iniciados e os espectros de IV e RMN obtidos até o momento coincidem com os encontrados em literatura. Testes de caracterização também foram obtidos para uma impureza cuja elucidação estrutural ainda está em andamento, e os resultados preliminares não se equivalem aos encontrados na literatura, apesar de algumas semelhanças.

Chemical characterization of lignocellulosic biomass for advanced biofuels production

https://proceedings.science/p/120613

Jussara Valente Roque [1]; Igor Gonçalves [2]; Josué Teixeira [3]; Marcio Henrique Pereira Barbosa [4]; João Carvalho [5]; Antônio Bonomi [5]; Luiz Peternelli [6]; Reinaldo Teófilo [3]

[1] UFV - Universidade Federal de Viçosa - Campus Viçosa; [2] Universidade Federal de Viçosa - UFV; [3] Universidade Federal de Viçosa; [4] Departamento de Agronomia / Universidade Federal de Viçosa; [5] (CNPEM) Centro Nacional de Pesquisa em Energia e Materiais; [6] Universidade Federal de Viçosa - Campus Viçosa

Extractives, insoluble and soluble lignin, and ashes determination were performed in energy cane, pine forest residues, and eucalyptus wood for evaluation to be used in advanced biofuels production.

Classificação de defeitos de grãos de café arabica por redes convolucionais desenvolvidas correlacionando aos seus perfis de carboidratos

https://proceedings.science/p/120548

Suzana Lucy Nixdorf [1]; William Bernardes Magalhães [2]

[1] Universidade Estadual de Londrina; [2] Departamento de Química /Centro de Ciências Exatas / Universidade Estadual de Londrina

Two convolutional networks were trained on coffee beans images aiming to locate and classify defective grains. Defects were also distinguished according to their carbohydrate profiles analyzed by HPLC

Colorimetric determination of Cl content in fuels using field-portable smartphone and USB camera: challenges and possibilities

https://proceedings.science/p/119888

Paola de Azevedo Mello [1]; Alice Penteado Holkem [1]; Gabrielle Dineck Iop [1]; Juliano Smanioto Barin [1]; Monica Voss [1]; Sandra Kunde Schlesner [1]; Adilson Ben Costa [2]; Gilson Helfer [2];

[1] Universidade Federal de Santa Maria; [2] Universidade de Santa Cruz do Sul

The presence of salt (expressed as chloride) in crude oil depends on the origin and of the wells production. If not removed, they can react to form a corrosive hydrochloric acid during the refining process, leading to operational problems as corrosion, incrustation and also in the deactivation of catalysts. Therefore, many analytical techniques or industry standard methods are routinely used to determine chloride in crude oil and fuels. Regardless of the analytical method, some aspects can be considered, such as: cost, time and analytical frequency. In this context, the colorimetric analysis using PhotoMetrix app can be an approach easily performed with low-cost, portable instrumentation and high analytical frequency. The present work proposes the extraction of chloride from the fuel to an aqueous phase, followed by colorimetric quantification of silver chloride using digital images. For that, parameters for extraction (the sample mass, the time, the temperature, the type and use of solvent, and the use of demulsifier and its concentration,) and for detection (the ratio between silver nitrate and indicator, lighting, the volume inside the vial, the focal distance, the number of pixels and the effect of pH) were evaluated. To obtain the digital images, an USB camera was placed in an open source 3D-printed chamber illuminated by a white light-emitting diode (LED) with light intensity controlled (Fig. 1). Sample and reagents (silver nitrate and the indicator) were added to an Eppendorf vessel, which was placed inside the chamber. Thus, the digital images were captured and converted into red, green, and blue (RGB) histograms, and partial least squares regression (PLS) models were used within the app. The PLS regression results (obtained directly from the app) were evaluated in terms of the number of samples and factors, the coefficient of determination (R2), the root mean squared error of calibration (RMSEC), the root mean squared error of cross validation (RMSECV), and the root mean squared error of prediction (RMSEP). The calibration curve (from 100 to 500 mg L-1 of Cl) was obtained using a PLS model with a R2 higher than 0.99. No significant differences ($p < 0.05$) between the measured and predicted values were identified. The RMSEC, RMSECV and RMSEP of PLS model were of 9.04, 31.2 and 26.1 mg L-1, respectively. **Figure 1** - Source 3D-printed chamber equipped with USB camera and, in detail, sample introduction. The presence of salt (expressed as chloride) in crude oil depends on the origin and of the wells production. If not removed, they can react to form a corrosive hydrochloric acid during the refining process, leading to operational problems as corrosion, incrustation and also in the deactivation of catalysts. Therefore, many analytical techniques or industry standard methods are routinely used to determine chloride in crude oil and fuels. Regardless of the analytical method, some aspects can be considered, such as: cost, time and analytical frequency. In this context, the colorimetric analysis using PhotoMetrix app can be an approach easily performed with low-cost, portable instrumentation and high analytical frequency. The present work proposes the extraction of chloride from the fuel to an aqueous phase, followed by colorimetric quantification of silver chloride using digital images. For that, parameters

for extraction (the sample mass, the time, the temperature, the type and use of solvent, and the use of demulsifier and its concentration,) and for detection (the ratio between silver nitrate and indicator, lighting, the volume inside the vial, the focal distance, the number of pixels and the effect of pH) were evaluated. To obtain the digital images, an USB camera was placed in an open source 3D-printed chamber illuminated by a white light-emitting diode (LED) with light intensity controlled (Fig. 1). Sample and reagents (silver nitrate and the indicator) were added to an Eppendorf vessel, which was placed inside the chamber. Thus, the digital images were captured and converted into red, green, and blue (RGB) histograms, and partial least squares regression (PLS) models were used within the app. The PLS regression results (obtained directly from the app) were evaluated in terms of the number of samples and factors, the coefficient of determination (R2), the root mean squared error of calibration (RMSEC), the root mean squared error of cross validation (RMSECV), and the root mean squared error of prediction (RMSEP). The calibration curve (from 100 to 500 mg L-1 of Cl) was obtained using a PLS model with a R2 higher than 0.99. No significant differences ($p < 0.05$) between the measured and predicted values were identified. The RMSEC, RMSECV and RMSEP of PLS model were of 9.04, 31.2 and 26.1 mg L-1, respectively. **Figure 1** - Source 3D-printed chamber equipped with USB camera and, in detail, sample introduction.

Comparative study employing the inline preparation for the determination of anions and cations by Ion Chromatography in industrial effluents

https://proceedings.science/p/120551

Camila da Silva Freitas Ribeiro [1]; Lucas Henrique Rhozier Simoes [2]; Arthur Santana da Silva [1]; Alex de Aguiar Novo [1]; Simone Chiapetta [1]; Laís Ferreira de Castro [1]

[1] Instituto Nacional de Tecnologia (INT); [2] Instituto Nacional de Tecnologia (INT); Universidade Federal Fluminense (UFF)

The sample preparation in-line of industrial effluents is more adequate than filtration.
Dialysis is an effective strategy to the analysis of anions and cations in industrial effluents.

Comparison study of the techniques of Total Reflection X-Ray Fluorescence Spectrometry (TXRF) and Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) for determining metals in na environmental sample

https://proceedings.science/p/120466

Luane Souza Silva Lage [1]; Alex de Aguiar Novo [1]; Arthur Santana da Silva [2]; Laís Ferreira de Castro [1]; Ana Paula Rodrigues [3]; Wilson Thadeu Valle Machado [4]

[1] DIQAN / Instituto Nacional de Tecnologia / Instituto Nacional de Tecnologia; [2] Instituto Nacional de Tecnologia; [3] Instituto de Biologia Marinha/Universidade Federal do Rio de Janeiro; [4] Departamento de Geoquímica/Universidade Federal Fluminense

The TXRF technique demonstrated a great advantage over ICP-OES for Pb analysis in environmental samples.

Conventional ESI versus Low-flow ESI Probe: moving toward directly coupling of SPME to MS/MS to determine Alzheimer's disease biomarkers

https://proceedings.science/p/120541

Israel Donizéti De Souza [1]; Caroline Fernandes Grecco [1]; Maria Eugenia Queiroz Nassur [1]

[1] Universidade de São Paulo

(I) Simple setup and robust option for bioanalytical applications; (II) Stable electrospray ion current for low-flow ESI probe; (III) Improved sensitivity for low-flow chromatography.

Desafios na determinação de elementos traço em amostras ambientais

https://proceedings.science/p/120696

Maria Tereza Carneiro [1]

[1] UFES

Essa apresentação visa abordar os desafios encontrados na determinação de elementos traço em amostras ambientais. Será abordados aspectos na análise de água do mar por ICP-MS, onde serão apresentados os problemas encontrados e as estratégias analíticas usadas para solucioná-los. Aspectos relacionados às dificuldades encontradas na análise de elementos traço também serão abordadas. Esses desafios apresentados indicam que as possibilidades de pesquisa nas análise de amostras ambientais ainda são muitas, visando o estabelecimento de resultados que de fato reflitam a situação do ambiente e permitindo um monitoramento do teor de elementos traço apropriado e confiável.

Desenvolvimento de métodos de decomposição em sistemas fechados para análise elementar de amostras de queijo branco

https://proceedings.science/p/119957

Allana Sobrinho dos Santos [1]; Pietra Strauch [1]; Rodolfo de Melo Magalhães Santana [1]; Maria G. A. Korn [1]
[1] Universidade Federal da Bahia

- Optimization step was performed using a full factorial design. - Conductively heated and microwave-assisted decompositions using diluted nitric acid were investigated.

Desenvolvimento de um novo polímero híbrido bifuncional para pré-concentração de diuron em meio aquoso

https://proceedings.science/p/120513

Daniel Morais Nanicuacua [1]; César Tarley [2]
[1] Universidade Estadual de Londrina/Universidade Púnguè; [2] Universidade Estadual de Londrina

New synthesis strategy combining two monomers, result in a material with good chemical and physic stability and high adsorption capacity. This can uptakes effectively diuron from aqueous medium.

Desenvolvimento e validação de métodos para determinação de impurezas em oxigênio medicinal e produção de materiais de referência gasosos

https://proceedings.science/p/120481

Vanderléa Souza [1]; Cristiane Augusto [1]; Andreia Fioravante [1]; Daiane Cunha [2]
[1] Instituto Nacional de Metrologia, Qualidade e Tecnologia; [2] Merck, Sharp & Dhome

This work presents the development and validation of the analytical methods used in the determination of impurities in medical oxygen, providing tools to prove the effectiveness of the proposed.

Determinação de cloro, ferro, e silício em cervejas por espectrometria de absorção atômica de alta resolução com fonte contínua e forno de grafite

https://proceedings.science/p/120603

Lais de Novaes Pires [1]; Jorge Almeida [1]; Fábio de Souza Dias [1]; Leonardo Sena Gomes Teixeira [1]
[1] Universidade Federal da Bahia

- HR-CS GF AAS and HR-CS GF MAS was used for the analysis of beer.
- Sequential and simultaneous strategies were used for the analysis by HR-CS GF AAS/MAS.
- The method allowed for the determination

Determination of bisphenol A and phthalates in utensils and toys for infants using HPLC-UV and bioaccessibility study

https://proceedings.science/p/119430

Gabriel Lima [1]; Ana Paim [2]; André Lavorante [1]
[1] Departamento de Química - Universidade Federal Rural de Pernambuco; [2] Departamento de Química Fundamental - Universidade Federal de Pernambuco

Bisphenol A and phthalates are endocrine disruptors.
The phthalate concentration is below the limits established by ANVISA.
DBP migration values were detected above those allowed by ANVISA

Determination of Ca, K, Mg and Na in sports supplements employing chemometrics tools and direct solid analysis by Laser-Induced Breakdown Spectroscopy (LIBS)

https://proceedings.science/p/120021

Diego Victor De Babos [1]; Fernanda Costa Pinheiro [2]; Bruna Soares Dionizio [2]; Edenir Rodrigues Pereira Filho [2]
[1] Universidade Federal de São Carlos; [2] UFSCar

Sports supplements as whey protein contain high protein content and are widely used by high-performance athletes and practitioners of physical activities for muscle regeneration. These supplements may also contain high concentrations of macronutrients such as Ca, K, Mg and Na, which play important physiological functions and therefore must be monitored to maintain a good functioning of the metabolism of users.1 LIBS, is an analytical technique that enables qualitative and quantitative fast analysis (<1 s), direct analysis or with minimal sample preparation and low generation of residues.2 Thus, new calibration strategies and chemometric tools were employed for the direct analysis of sports supplements using LIBS aiming at the determination of macronutrients Ca, K, Mg and Na. LIBS emission spectra of the analytes were obtained using an instrument model J200 (Applied Spectra, USA), with a Nd:YAG laser (1064 nm). Approximately 200 mg of each sample was used to obtain pellets using a press (70 kN for 2 min). A Doehlert factorial design with a central point was used to optimize the instrumental conditions for the analyte determinations, being evaluated delay time (0.8, 1.4 and 2 µs) and laser pulse fluence (368, 1422, 2476, 3530 and 4584 mJ cm-2) variables. The following emission lines were monitored: Ca (393.36 and 396.84 nm), K (766.49 and 769.89 nm), Mg (383.83 and 518.36 nm) and Na (588.99 and 589.59 nm), then overall desirability (using signal-background ratio for all wavelengths) was calculated and used as design response. The final instrumental conditions were delay time of 1.4 µs and fluence of 2476 mJ cm-2. Approximately 200 spectra (n = 3) were obtained for each sample, and twelve modes of spectral normalization were evaluated. All sports supplements were also analyzed by ICP OES to obtain reference values to assess the accuracy of direct determinations by LIBS. The concentrations determined by ICP OES were in the range of 3351 to 7069 mg kg-1 Ca, 3870 to 13639 mg kg-1 K, 626 to 2678 mg kg-1 Mg and 1293 to 5170 mg kg-1 Na. Three calibration strategies were evaluated for direct determination by LIBS: 1- matrix-matching calibration (MMC),3 2- one-point and multi-line calibration (OP MLC),4 and 3- single sample calibration (SSC).5 For the determination of Ca, MMC, OP MLC and SSC presented good values of trueness (68 to 119%) and RSD (2 to 30%). For K, OP MLC enabled the best trueness values (87 to 102%) and RSD (1 to 10%), except for some samples. For Mg, good trueness values (83 to 120%) and RSD (1 to 14%), with the exception of some samples, were obtained using MMC and OP MLC. For Na only using SSC presented reliable values for trueness (79 to 116%) and RSD (4 to 10%), for most samples. Unsatisfactory values of trueness were obtained for some elements in some samples due to the strong matrix effects in the LIBS determination. However, some calibration strategies evaluated were able to overcome or minimize the matrix effects for most determinations. The use of principal component analysis - PCA and LIBS spectra made it possible to observe two clusters of samples: high and low protein content in sports supplements. Fast, direct and green method is developed for the determination of macronutrients in sports supplements (whey protein) using LIBS. [1] F.K. Haraguchi et al., Rev. Nutr., 19(4) (2006) 479-488. [2] V.C. Costa et al., Quim. Nova, 42(5) (2019) 527-545. [3] D. V. Babos et al., Spectrochim. Acta B, 155 (2019) 90-98. [4] Z. Q. Hao et al., Opt. Express, 26 (2018) 22926. [5] R. Yan et al., Anal. Chim. Acta, 1064 (2019) 11-16.

Determination of piceatannol from passion fruit seeds (Passiflora edulis Sims “Flavicarpa”) using a modified QuEChERS method and HPLC-DAD

https://proceedings.science/p/120503

Liane Maldaner [1]; Ana Paula Lourenção Zomer [1]; Carina Alexandra Rodrigues [1]; Eliza Mariane Rotta [1]; Jesui Visentainer [1]

[1] Universidade Estadual de Maringá / Programa de Pós-Graduação em Química / Departamento de Química

QuEChERS method was successfully applied to piceatannol determination from passion fruit seeds.

Passion fruit seeds showed a high concentration of piceatannol.

Determination of trace elements in liver and muscle of tunas of the species Katsuwonus pelamis by mass spectrometry with inductively coupled plasma.

https://proceedings.science/p/120762

Roberto Carlos Fernandes Barsotti [1]; Heloisa França Maltez [1]

[1] Universidade Federal do ABC

Trace elements determination in tunas by ICP-MS. Tissue related diferences.

Developing a LC-MS/MS method to determine amyloid ß peptides in plasma samples obtained from patients with Alzheimer’s Disease

https://proceedings.science/p/120681

Caroline Fernandes Grecco [1]; Israel Donizéti de Souza [1]; Maria Eugenia Queiroz Nassur [1]

[1] Universidade de São Paulo

(I) Determination of amyloid β peptide in plasma sample from patients with Alzheimer’s Disease. (II) Development of an ultra-high performance liquid chromatography tandem mass spectrometry method.

Development of a LC-MS/MS method for simultaneous quantification of carbidopa, levodopa, and their metabolites in human plasma

https://proceedings.science/p/120549

Lidia Miranda da Silva [1]; Israel Donizéti de Souza [1]; Caroline Fernandes Grecco [1]; Maria Eugenia Queiroz Nassur [1]

[1] Universidade de São Paulo

• MS/MS parameters and chromatographic conditions (HILIC mode) were optimized;
• DPX (MCX Oasis® sorbent phase) provided good extraction efficiency to concentrate the studied analytes.

Development of a miniaturized QuEChERS method for the extraction of phenolic compounds in red pepper (Capsicum baccatum L.)

https://proceedings.science/p/120757

Liane Maldaner [1]; Carina Alexandra Rodrigues [1]; Ana Paula Lourenção Zomer [1]; Jesui Visentainer [1]

[1] Universidade Estadual de Maringá / Programa de Pós-Graduação em Química / Departamento de Química

• µ-QuEChERS used ten times less sample amount, extraction solvents and partition salts and two times less clean-up sorbents; • µ-QuEChERS successfully extracted phenolic compounds from red peppers.

Development of a paper-based analytical device for ranitidine determination

https://proceedings.science/p/119522

José Guimarães Ferreira de Lima Júnior [1]; Allysson Roberto Barbosa de Lima [1]; Elvis Max Xavier de Lima [1]; Fabiane Caxico [1]; Diógenes Meneses [1]

[1] Universidade Federal de Alagoas

A new PAD for ranitidine colorimetric detection based on its derivatization reaction with NBD-Cl. The proposed method is simple, affordable and ease to use.

Development of a practical and effective dispersive micro-solid phase extraction procedure for the determination of 42 multiclass pesticides in water samples

https://proceedings.science/p/119477

Madson Nascimento [1]; Gisele Olimpio da Rocha [1]; Jailson Bittencourt de Andrade [2]

[1] Universidade Federal da Bahia; [2] SENAI CIMATEC

A practical D-μ-SPE procedure combined with a fast micro-desorption step was developed. The experimental design was employed in the optimization of the extraction conditions.

Development of an analytical method for crude oil digestion and metals determination by ICP-OES

https://proceedings.science/p/119881

Jussiane Souza da Silva [1]; Mariele Samuel do Nascimento [1]; Gabriel T. Druzian [1]; Rochele S. Picoloto [1]; Paola A. Mello [2]; Erico M. M. Flores [1];

[1] UFSM; [2] Universidade Federal de Santa Maria

Crude oil is commonly found in reservoirs associated with sedimentary rocks. It is a hydrocarbon-based matrix, containing some elements, such as sulfur, nitrogen, oxygen and metals (e.g, Ni, V, Na, Ca and others). Regarding to the metals presence in crude oil, it is well known that their concentration depends on the type of geological formation, location as well as age and depth of reservoir.1 The presence of metals in crude oil may cause poisoning, corrosion, and affect equipment during crude oil refining process, even at low concentration.1 However, taking into account the difficulties for crude oil digestion and the low levels of same contaminants typically found in crude oil, as well as the low carbon content and low acidity required in digests to use plasma-based techniques, the development of an accurate sample preparation is necessary. In this work, crude oil decomposition was performed using microwave-assisted wet digestion in a pressurized digestion cavity (MAWD-PDC)2 for the determination of Ba, Ca, Fe, K, Li, Mg, Na, Ni, Sr and V by inductively coupled plasma optical emission spectrometry (ICP-OES). A high-pressure microwave-assisted digestion system (Multiwave 7000, Anton Paar, Austria) equipped with five quartz vessels (80 mL), with maximum temperature and pressure of 270 °C and 160 bar, respectively, was used. The metals and carbon determination were performed by an ICP-OES equipment (Optima 4300DV, Perkin Elmer, USA). The determination of the residual acidity was performed by titration (836, Metrohm, Switzerland). Operational conditions, such as the sample mass (0.5 to 1.2 g), the volume of HNO3 (6, 8, and 10 mL), the maximum temperature (220, 250, and 270 °C), and microwave irradiation time (5, 10, 15, and 20 min) were investigated. Using the optimized conditions (8 mL of 14.4 mol L-1 HNO3, 270 °C and 20 min), the MAWD-PDC method allowed the digestion of 1.2 g of crude oil, resulting in a very low limit of quantification (from 0.10 to 0.52 μg g-1). The proposed method was applied to four oil samples and the carbon content and residual acidity in digests were about 3.5 g L-1 and 10%, respectively. No statistical difference was observed between the results obtained by ICP-OES after MAWD-PDC and the certified values of certified reference material (NIST 1634c, fuel oil). The proposed method was suitable for the determination of Ba, Ca, Fe, K, Li, Mg, Na, Ni, Sr and V at ultra-trace levels in crude oil and it can to be used for routine analysis in the petroleum industry.
1. J.G. Speight. Handbook of Petroleum Analysis, John Wiley and Sons Inc, New Jersey, 2001, 519 pp. 2. Anton Paar, Instruction Manual and Safety information, Multiwave 7000, 43 pp.

Development of an analytical method for determination of minerals in peels and pulps of peach fruits by MIP OES

https://proceedings.science/p/119509

Mariana Antunes Vieira; Ana Renata da Rosa Louzada [1]; Letícia de Oliveira Oliz [1]; Anderson Schwingel Ribeiro [1]
[1] Universidade Federal de Pelotas

The city of Pelotas, located in the southern region of the state of Rio Grande do Sul stands out in the cultivation of peach, being considered the largest national producer of peaches for industry and fresh consumption. Studies show that, in general, peels of fruits have more nutrients than pulps. However, to have an adequate supply of macro and micronutrients, according to the Recommended Daily Intake (RDI), it is essential to determine the concentration of elements in the peels and pulps of fruits. Thus, this work presents the development of an analytical method to determine the concentration of minerals such as Ca, Cu, Fe, K, Mg, Mn, Na and Zn in peel and pulps of peach, comparing them with nutritional composition. Samples of four peach cultivars, produced in the Pelotas Region (BR-3, Tourmaline, Dourado-1 and BRS Libra) were analyzed. The determinations were performed by microwave-induced plasma optical emission spectrometry (MIP OES) technique. The peels and pulps were separated and triturate before analysis. For sample preparation was employed a digester block with reflux system using the following conditions: 500 mg of sample was weighed into a glass digester tube, and 5.0 mL of 9 mol L-1 HNO3 was added. The mixture was heated in a digester block at 135 °C for 3h. The tubes were removed from digester block and after cooling, 2 mL of H2O2 was added and the tubes were taken again to the digester block to finish the decomposition (1 h at 120 °C). Under these conditions, the parameters of acidity and total dissolved solids were within the limits established by the manufacturer of the MIP OES spectrometer. Also, the residual carbon also was determined and the obtained value (1.6% (m/m)) demonstrated the sample decomposition efficiency. The accuracy was evaluated through the analysis of certified reference material (CRM-Agro C1004a of tomato pulp) and recovery tests. The levels of minerals in the peels and pulps of peach were close for all cultivars analyzed, with no statistically significant difference. The profile of minerals in the peels showed that the concentrations of the elements investigated were higher than those found in the pulps: Ca (95 and 50 mg kg-1), Cu (1.34 and 0.97 mg kg-1), Fe (5.6 and 2.8 mg kg-1), Mg (142 and 95 mg kg-1), Mn (1.97 and 1.20 mg kg-1), Na (72 and 54 mg kg-1) and Zn (1.90 and 1.80 mg kg-1), respectively. Potassium showed the highest concentrations in all samples, with values in the peels and pulps of 1719 and 1549 mg kg-1, respectively. Copper was the element with the greatest contribution to the recommended daily intake, being able to supply 15% of the RDI value in the peels and 11% in the pulps, for 100 g of edible portion, followed by the others with contents less than 10%. The developed method was efficient for the determination of the minerals in peels and pulps of peach fruits, with no statistically significant differences between the cultivars analyzed; it was also proved that the peels have higher levels of essential minerals than the pulps.4 It follows that removal of peel from peach fruits may induce significant nutrient losses and because of that, the intake of fruits along with their peels can be more beneficial as a potential source of high-value components.

Development of methodology for cadmium extraction and preconcentration using aqueous two-phase system

https://proceedings.science/p/119896

Dilaine Suellen Caires Neves [1]; Anderson Santos Souza [2]; Leandro Rodrigues de Lemos [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Universidade Federal da Bahia

Methodology for cadmium determination that fits the principles of green chemistry. Extraction and preconcentration without the use of extractor agent.

Direct determination of contaminants in milk long-life packaging by mass spectrometry

https://proceedings.science/p/120638

Daniel de Almeida Soares [1]; Igor Pereira [1]; Rosy Simas [2]; Boniek Gontijo Vaz [1]; Andréa Rodrigues Chaves [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal do Rio de Janeiro

This work presents a semi-quantification study of Bisphenol (A and S) in long-life milk packaging using an ambient mass spectrometry technique.

Dispersive liquid-liquid microextraction based on solidification of floating organic droplet in the extraction of carbofuran

https://proceedings.science/p/119996

Giovana Pedrina [1]; Wanessa Melchert Mattos [2]

[1] Escola Superior de Agricultura "Luiz de Queiroz" (ESALQ) - Universidade de São Paulo (USP); [2] Universidade de São Paulo

Solidification of floating organic droplet in dispersive liquid-liquid microextraction as a clean analytical implement

Development of a green analytical procedure for extraction of pesticide

Dispersive Liquid-Liquid Microextraction for total Sulfonamides in Bovine Milk Samples

https://proceedings.science/p/119563

Lais Alves Maroubo [1]; Wanessa Melchert Mattos [2]

[1] Escola Superior de Agricultura "Luiz de Queiroz" / Universidade de São Paulo / Departamento de Ciências Exatas; [2] Universidade de São Paulo

Development of a fast, economical and clean analytical method for extraction and preconcentration of total sulfonamides in bovine milk samples based on the Dispersive Liquid-Liquid Microextraction.

Electroanalytical method for the quantification of the carbamate pesticide aldicarb (chumbinho) using a modified gold electrode

https://proceedings.science/p/119985

Severino Marcelino dos Santos Neto [1]; Elton Filipe Tenório de Lima [2]; Márcio Vilar França Lima [3]; Frederico Duarte de Menezes [3]; Thiago Regis Longo César da Paixão [4]; Thiago Matheus Guimarães Selva [5]

[1] Universidade Federal Rural de Pernambuco; [2] Universidade Federal de Pernambuco; [3] Instituto Federal de Educação, Ciência e Tecnologia de Pernambuco ; [4] Universidade de São Paulo; [5] Instituto Federal do Rio de Janeiro

Pesticides are chemical compounds used in agriculture to combat or prevent unwanted pest infestations. Its importance has generated many discussions nowadays due to the fact that the latest scientific research has been pointing out that these can cause diseases such as cancer. One of the most used classes of pesticides are carbamates, which may highlight aldicarb, which is popularly known as “chumbinho”. Its marketing has been banned in Brazil since 2012, however, it is used as a rodenticide and in criminal practices such as homicides and suicides. Therefore, the development of reliable, simple and low-cost analytical methods for monitoring this type of substance is of fundamental importance. Electroanalytical techniques use electrical properties of chemical species that can be measured. Within this branch, we can highlight voltammetric techniques, a set of electroanalytical techniques that measure the electric current of electron transfer processes between a chemical species and the surface of an electrode. In these instrumental techniques, a working electrode, an auxiliary and a reference electrode are used. Working electrodes can be modified in order to improve their sensitivity and / or selectivity in the detection of certain chemical species. In this work, the gold electrode was modified to produce a gold nanoporous film, which made it possible to detect the aldicarb pesticide. This modification occurs through the oxidation of gold in a strongly acidic medium at high potentials and subsequent reduction. The nanoporous film produced has a high surface area, allowing better electron transport when compared to gold electrodes without this modification. Figure 1 shows the comparison of the cyclic voltammetric response of the aldicarb on gold bare and gold modified electrodes. In view of the versatility, low cost and excellent sensitivity of voltammetric techniques, an analytical method was developed using differential pulse voltammetry to quantify aldicarb. At first, experimental variables were studied to optimize the method, such as pH, support electrolyte, gold electrode modification time and analyte pre-concentration time. After optimizing these parameters, an analytical curve was constructed with a concentration range between 0.20 to 2.64 µmol L−1 (R2 = 0.9806), and a detection limit of 18 nmol L−1 and standard deviation relative less than 1%. Therefore, the proposed method has excellent sensitivity and reproducibility, which makes it promising to be used in routine laboratories and in the field.

Electromembrane extraction (EME) method for the multi-class pesticides determination in soil samples

https://proceedings.science/p/120452

Rafael Oliveira Martins [1]; Giovanna Lopes [1]; Carla Santos de Freitas [1]; Rosy Simas [2]; Boniek Gontijo Vaz [1]; Maria Eugenia Queiroz Nassur [3]; Andréa Rodrigues Chaves [1]
[1] Universidade Federal de Goiás; [2] Universidade Federal do Rio de Janeiro; [3] Universidade de São Paulo

EME was successfully used to the extraction of 13 multi-class pesticides
An effective methodology for pesticides extraction has been developed
The EME parameters were evaluated and optimized

Enantioselective chromatographic separation of the fungicide penconazole

https://proceedings.science/p/119862

Maike Felipe Santos Barbetta; Icaro Salgado Perovani [1]; Anderson Rodrigo Moraes de Oliveira [1]
[1] FFCLRP-USP

Penconazole is a systemic chiral fungicide applied mainly in grape, apple, tomato and cucumber to control powdery mildew. Its application is carried out by spraying the leaves with an emulsion of the racemic mixture of the pesticide. Recent studies have indicated an increase in the concentration of this pesticide in water and food, thus increasing the risk of contamination in non-target organisms, such as humans. It's also known that penconazole can exhibit enantioselective degradation and toxicity in some species. Therefore, more efficient analysis methods that take into account the chiral character of this compound are necessary. This work aims to develop a new enantioselective chromatographic method to analyze the chiral fungicide penconazole. Seven different columns with different chiral selectors, different particle diameters as well as length were evaluated (Chirobiotic V®; Chirobiotic T®; Chiralpak ADRH® and AD-3®; Chiralcel OD-H® and OD-3®; Chiralcel OJ®; Lux Cellulose 1® and Lux Cellulose 2®) in polar organic mode (100% acetonitrile, methanol or ethanol) and in reversed phase (70:30 v/v mixtures of acetonitrile, methanol or ethanol and water) modes of elution. The resolution values between the enantiomers were below 1.5 for all the chiral columns evaluated employing the polar organic modes. Good separation (resolution ≥ 1.5) was obtained using the Chiralpak AD-RH® column with methanol: water, and both Chiralcel OD-H® and OD-3® column by employing methanol: water and ethanol: water as mobile phases. Analysis time varied from 10 to 30 minutes. The best condition for the enantiomeric separation was obtained with Chiralcel OD-3® column by using ethanol: water (70:30 v/v) as mobile phase, in which the resolution was 1.9 and the total analysis time was 10 minutes.

Espectroscopia de fluorescência combinada com métodos de classificação multivariada para detectar adulteração em mel de Aroeira

https://proceedings.science/p/120412

Daphne Antônio [1]; Débora Sampaio [2]; Bruno Botelho [2]; Marcelo Martins de Sena [2]
[1] Universidade do Estado de Minas Gerais; [2] Universidade Federal de Minas Gerais

Aroeira honey samples adulterated with polyfloral honey
Models built with spectrofluorimetric data and multi-way classification methods
Environmentally friendly method with potential to routine use

Estratégias analíticas de preparo de amostras usando ácido orgânico para análise elementar

https://proceedings.science/p/120701

Kelly G. Fernandes Dantas [1]
[1] Universidade Federal do Pará

Estratégias de calibração via "one-point" e compatibilização de matriz para a quantificação de elementos potencialmente tóxicos em amostras de madeira via LA-ICP-MS

https://proceedings.science/p/120468

Danielle S Francischini [1]; Marco A.Z. Arruda [1]

[1] Universidade Estadual de Campinas

Different calibration strategies in LA-ICP-MS were compared and validated. Pb, Cd, Ni and Ba were quantified in SRM sample with recovery > 71%. These methods can be applied in imaging via LA-ICP-MS.

Estudos biofísicos de interação para avaliação do mecanismo de inibição da urease por um benzilisotiocianato natural

https://proceedings.science/p/119459

Maria Célia Tavares [1]; Josué Carinhanha Caldas Santos [1]; Carlos J. A. Silva-Filho [2]; Jair Mafezoli [2]; Francisco G. Barbosa [2]; Maria da Conceição Ferreira de Oliveira [2]; Carolina Raquel Said Dau Gonçalves [3]; Luzia Valentina Modolo [3]; Ângelo de Fátima [3]

[1] Universidade Federal de Alagoas ; [2] Universidade Federal do Ceará ; [3] Universidade Federal de Minas Gerais

A urease é uma enzima que catalisa a degradação da ureia em NH3 e CO2. No solo, sua ação leva a perdas de nitrogênio (N) por volatilização (30-70%), pois a ureia é o principal fertilizante nitrogenado empregado em diferentes culturas. A adição de inibidor de urease à ureia é uma alternativa que reduz em até 60% as perdas de N por volatilização. Nesse sentido, estudos biofísicos para avaliar o potencial inibidor de compostos frente a urease são importantes para aplicação biotecnológica pois, atualmente, o tiofosfato de N-(n-butil)-triamida (NBPT) é o único inibidor comercial de urease para fins agrícolas. Assim, esse trabalho tem como objetivo avaliar o mecanismo de inibição da urease pelo 4-(4'-O-acetil-α-L-ramnoseoxi)benzilisotiocianato (MFC) isolado das flores de Moringa oleifera Lam (Moringaceae) por Almeida et al. (2017). Foram realizados estudos cinéticos e de inibição enzimática (Brito et al. 2012). Foi monitorada a fluorescência intrínseca da urease por fluorescência normal e os resíduos de tirosina e triptofano empregando fluorescência sincronizada. Foram realizados ensaios específicos para monitorar grupos amino e tiol livres na ausência e na presença do ligante por UV-vis e fluorescência molecular, bem como ensaio de níquel e espectrometria de massas. Os estudos enzimáticos indicaram que MFC é um inibidor misto com atividade inibitória (IC50 = 0.487 mM) comparada a outros compostos contendo enxofre (captopril IC50 = 0,523 mM e bitionol IC50 = 0,376 mM). Os estudos por UV indicaram possíveis alterações conformacionais na enzima decorrentes da interação com o MFC. A partir da titulação espectrofluorimétrica obtiveram-se os valores de Ksv (1300 M-1) e Kb (180 M-1), que refletem a magnitude da supressão de fluorescência e da ligação entre a urease e o MFC, enquanto o valor n (0,77) próximo a 1 indica que a estequiometria do complexo é 1:1. Além disso, houve supressão de fluorescência com o aumento da concentração do MFC no monitoramento dos resíduos de Tyr e Trp, reforçando a atuação do MFC como inibidor misto, pois os resíduos Trp495 e Trp648 estão distantes do sítio catalítico (BRAGA et al., 2019).Os resultados obtidos indicam que MFC interage com a urease e apresenta-se como um derivado natural promissor para aplicações biotecnológicas como inibidor de urease.

Estudos preliminares para determinação de mercúrio em sedimento marinho por ICP-MS e CV-ICP-MS

https://proceedings.science/p/120553

Carolina Scocco Provete [1]; Bruna Dalfior [1]; Rafael Mantovaneli [1]; Maria Tereza Carneiro [2]; Geisamanda Pedrini Brandão [1]

[1] Universidade Federal do Espírito Santo; [2] UFES

Determination of mercury in marine sediment. Cold vapor and ICP-MS analysis.

Evaluation of chemical attributes in soil of black pepper cultivation from ES - Brazil using chemometrics

https://proceedings.science/p/119437

Merisnet Ferde [1]; Nathalia Wyatt [1]; Gabriely Folii [1]; Geisamanda Pedrini Brandão [1]; Vinicius Câmara Costa [1]; Paulo Roberto Filgueiras [2]; Maria Tereza Carneiro [1]

[1] UFES; [2] Ufes

Trace elements in soil of black pepper cultivation. Physical chemical characterization of the soil of black pepper cultivation. Chemometrics analysis

Evaluation of direct interaction between amino acids and glutathione coated CdTe quantum dots and potential application in urinalysis

https://proceedings.science/p/120089

Leila Santana Viana Barbosa [1]; Rodolfo de Melo Magalhães Santana [1]

[1] Universidade Federal da Bahia

Amino acids (AA) have been determined employing quantum dots (QD) as photoluminescent probes for indirect sensing, based on AA-quencher complexation at turn-off-turn-on approaches1,2. The present work aims to evaluation of direct AA sensing by QD and its potential for fast urine analysis. Preliminary assays, using glutathione-coated CdTe QD (GSH-CdTe), were performed against three amino acids groups divided according to their side chains. It was observed that AA with a positive charge or neutral polar chains, namely L-histidine (His) and L-threonine (Thr), promoted a luminescence quenching up to 90% in the GSH-CdTe. Studies on the His-QD binding and quenching mechanism indicated the occurrence of static quenching with the complex association constant (Ksv) varying from 28.1 to 9.7 L/mol due to increasing temperature. Thermodynamic parameters were determined by van't Hoff equations, estimating values of ΔH = -76.5 kJ/mol, ΔS = -227.4 J/K mol and ΔG from -9.8 until -6.4 kJ/mol at 20 to 35 °C. In addition, no variation of Ksv (ΔKsv < 11%) was observed due to the changes in the ionic strength indicating preferentially interactions by Van der Waals forces and/or hydrogen bonding. The evaluation of the interaction parameters showed that in ammoniacal buffer (0.25 mol/L) at pH 8.0, the QD nanocrystal of 2.2 nm responded only to His with LOD of 1.6x10-4 mol/L. Determination of His was carried out on artificial and human urine with recoveries ranging from 78.7 to 127.6%.

Evaluation of matrix effect on the determination of metallic elements in artisanal minas cheese by flame atomic absorption spectrometry

https://proceedings.science/p/119651

Tercio P. F. Xisto [1]; Ana Carolina F. C. Borges [1]; Emylle E. Santos [1]; Roberta E. Santos Froes [1]; Emanueli do Nascimento da Silva [1]

[1] UFOP

Nowadays, milk and milk products are highlighted because of their nutritional value and protein amount, and among these dairy products, cheeses are taking up space in the Brazilian market. Therefore, the production, commercialization, and internationalization of Artisanal Minas Cheese grow more and more. However, there are still few studies dedicated to this type of food. Thus, the present study aimed to use a method of preparing the cheese sample using dissolution in alkaline medium in order to determine Cu, Mn, Fe, Zn, Mg, and Ca, as well as evaluating the matrix effect in the analyzes by Flame Atomic Absorption Spectrometry (F AAS). The method of preparing the cheese samples was the solubilization in alkaline medium using tetramethylammonium hydroxide (TMAH), which was previously optimized using a 2^4 experimental design. The fresh cheese samples were weighed (~ 1 g) directly into a 50 mL centrifuge tube. Then, 9.5 mL of triton x-100 solution in deionized water (~ 5% v/v) and 0.5 mL of TMAH 25% (w/v) were added. Subsequently, the tubes were taken to an ultrasound bath for 30 min at 50 °C, aiming at the solubilization of the matrix and extraction of the metallic elements. Finally, the samples were diluted and taken for analysis in flame atomic absorption spectrometry. For the analysis, the external calibration (dilution of the standards in water) and matrix-matched calibration curves were evaluated. The solutions obtained in the sample preparation were mixed to obtain a pool, which was used to prepare the matrix-matched curves at the appropriate dilutions for each element, 2x (Cu, Mn), 4x (Fe, and Zn), 20x (Mg), and 100x (Ca). The dilutions were chosen according to the concentration of the analytes in the samples and in the certified reference material (NIST 1846). To evaluate the possible matrix effect, the slopes of the external and matrix-matched curves were compared. The results showed that for Cu, Fe, and Zn there is a significant matrix effect because the slopes are more than 10% different among the curves.

However, it is possible to determine these elements if the matrix-matched calibration curve is used. Finally, for the other elements (Mn, Mg, and Ca), the variation was lower than 10%, then it is possible to use an external calibration curve to analyze the cheese samples.

Evaluation of sample treatment in micro-scale for determination of Ca, Cu, Fe, K, Mg, Na and Zn in sausage by MIP OES

https://proceedings.science/p/119510

Anderson Schwingel Ribeiro [1]; Ana Claudia B. Luckow [1]; Sabrina H. Scherdien [1]; Daisa H. Bonemann [1]; Charlie G. Gomes [1]; Yasmin Bloedorn [1]; Adriane M. Nunes [1]

[1] Universidade Federal de Pelotas

Sausage is an industrialized meat product obtained from the emulsion of beef, pork or poultry and edible offals, which attribute various nutrients and essential elements. During their processing, many sodium-based additives are used, which are responsible for preserving the food and enhancing the flavor, making the sausage a risky food for the population when consumed in excess due to the high concentrations of this element. In addition, the presence of elements that are beneficial to health, but in excess, can cause several disturbances in the physiological system. Due to the complexity of the sausage sample matrix, rich in fat, it is necessary studies for the correct sample preparation for analysis, to obtain accurate and precise results. The literature reports several methods for biological samples, which most often use large quantities of samples and reagents, associated with heating at high temperatures. Therefore, the micro-scale method is attractive, because in addition to reducing the amount of sample for analysis, it consumes lower volume of reagents, generating a smaller amount of waste, reducing the analysis time and offering greater security for the analyst. Thus, this study aimed to evaluate the acidic decomposition method in micro-scale, using mini vessels made of polytetrafluoroethylene (PTFE) for sample preparation in a closed system with microwave heating for determination of Ca, Cu, Fe, K, Mg, Na and Zn in sausage samples. The determinations were performed by microwave-induced plasma optical emission spectrometry (MIP OES) technique. The method developed was based on the studies carried out by Oliz et al.1 A mapping of the power distribution (W) was carried out inside the microwave oven, as described by Rosini et al.2 in order to decompose a larger number of samples simultaneously. Sausage samples were acquired in a local supermarket of Pelotas and were comminuted using a blender. The best conditions for micro digestion (mass, irradiation time, acid volume and microwave power) were optimized by employing a central composite design (CCD), at two levels.3 This way, 40 mg of sausage were weighed directly into mini vessels and was added 400 µL of HNO3. Then, the vessels were closed and placed in the microwave oven, using a rounded support with a capacity for six vessels. A beaker with deionized water was placed in the center of the support. The decomposition occurred in 3 min at level 7 (power of 475 W). The resulting solutions were transferred to polypropylene tubes and the final volume of 5.0 mL was completed with deionized water. The accuracy was evaluated through the analysis of certified reference material (SRM 1546 - meat homogenate) with good recoveries (80 to 117%) for all analytes. The method was applied for the analysis of a sausage sample. Sodium presented highest concentration (9108 ± 673 mg kg-1), followed by K (1364 ± 99 mg kg-1), Ca (604 ± 13 mg kg-1) and Mg (216 ± 19 mg kg-1). The analytes Cu, Fe and Zn presented close concentrations: 10 ± 0.8; 12 ± 0.7 and 12 ± 0.9 mg kg-1 , respectively. As conclusion, it was possible to perform simultaneous decomposition of the sausage samples using the sample treatment in micro-scale and the microwave oven, which provided an increase in the analytical frequency of the method. The procedure showed to be fast, safe and with lower consumption of reagents and samples, minimizing waste generation and the conventional microwave oven is easy to access, facilitating its use in routine analyzes.

EXTRAÇÃO OTIMIZADA E CARACTERIZAÇÃO MOLECULAR DE ÓLEO BETUMINOSO DE MATURE FINE TAILING (MFT).

https://proceedings.science/p/120536

Vinícius Matos da Costa [1]; Jhonattas Carregosa [1]; Jandyson Machado Santos [2]; Alberto Wisniewski Jr [3]

[1] Universidade Federal de Sergipe; [2] Universidade Federal Rural de Pernambuco; [3] Universidade Federal de Sergipe, Brasil.

An optimized extraction method capable of extracting 67% of Mature Fine Tailing oily fraction.
The acidic compound of O2 class are likely to be responsible for the high stability of the MFT emulsion.

Forensic Potentiality of Near-Infrared in the Geographical Discrimination of Tucumã Oil
https://proceedings.science/p/119575

Rosivaldo Ferreira de Sousa [1]; Francisco Panero [1]; Pedro dos Santos Panero [2]; Antonio Alves de Melo Filho [1]; João Panero [3]; Fernando Sérgio Escócio Drummond Viana de Faria [4]; Anselmo Fortunato Ruiz Rodriguez [4]
[1] Universidade Federal de Roraima; [2] Instituto Federal de Ciências e Tecnologia de Roraima; [3] IFRR; [4] Universidade Federal do Acre

Forensic Potentiality of Near-Infrared in the Geographical Discrimination of Tucumã Oil. The potential of NIR-infrared spectroscopy for geographical discrimination of oils from the fruits of tucumã.

Halogens and sulfur in nails: Single analysis using ion chromatography with suppressed conductivity and mass spectrometry afther combustion reaction
https://proceedings.science/p/119452

Diogo la Rosa Novo [1]; Priscila Tessmer Scaglioni [1]; Fernanda Pitt Balbinot [1]; Álisson Aline da Silva [1]; Romina Moreira [1]; Marcia Mesko [1]
[1] Universidade Federal de Pelotas

Halogens and sulfur were determined in human nails using a single analysis, and drawbacks of conventional analytical methods were overcome.

HPLC fingerprint and PARAFAC in a non-target analysis to evaluate organic grape juices
https://proceedings.science/p/120470

Leonardo Valderrama [1]; Bogdan Demczuk [2]; Patricia Valderrama [2]; Eduardo Carasek da Rocha [1]
[1] Universidade Federal de Santa Catarina; [2] Universidade Tecnológica Federal do Paraná

Organic grape juice evaluation through HPLC in a non-target way.
Chromatograms arranged in three-way arrays.
Multi-way decomposition with PARAFAC.
Loadings on the replicates mode resemble precision.

Identificação de adulterações no carvão ativado de osso utilizado para o tratamento de água de consumo humano por NIR-PLS-DA
https://proceedings.science/p/120487

Cristiane Pappis [1]; Roberta Oliveira Santos [2]; Gilson Augusto Helfer [3]; Valderi Luiz Dressler [1]; Edson Irineu Muller [1]; Adilson Ben da Costa [2]
[1] Universidade Federal de Santa Maria; [2] Universidade de Santa Cruz do Sul; [3] Universidade do Vale do Rio dos Sinos

Desfluoridation of public water supply. Adsorption of fluoride ions using bone activated coal. Adulterations identification using NIR-PLS-DA.

Identification and characterization of biological fluids in clothes by hyperspectral images
https://proceedings.science/p/119439

Pedro Augusto de Morais [1]; Camila Morandi Solva [2]; Mariana E. Pinheiro [3]; Pedro H. C. Naves [2]; Ana L. A. Calil [2]; Ana C. Humanes [2]; Eliude B. Gomes [2]; Diego Mendes de Souza [2]
[1] Universidade Federal de Goiás; [2] Instituto de Criminalística da Polícia Civil do Distrito Federal; [3] Universidade de Brasília

A nondestructive method based on hyperspectral images is proposed to identify and classify the biological fluids: blood, semen and vaginal fluid in clothes.

Identification and classification of CBC rifle projectiles by X-ray fluorescence in conjunction with multivariate analysis

https://proceedings.science/p/119579

Cristina Maria Barra [1]; Victor Gabriel de Paula Saide [2]; Jose Geraldo Rocha [2]; Matthieu Tubino [3]; Gustavo Shimamoto [3]; André Canuto [4]

[1] Universidade Federal Rural do Rio de Janeiro; [2] UFRRJ; [3] UNICAMP; [4] PCRJ

The origin of projectiles found at crime scenes is commonly identified by ballistic comparison. However, in processes involving a rifle, the projectile can be found deformed, making that comparison impossible. In this cases, lead fragments from projectiles can be explored to assess the possibility of a link between the crime scene, the projectile and the suspect1. In this work, an exploratory analysis of the chemical composition of the core of rifle projectiles was carried out, determined by X-Ray Fluorescence by Sequential Wavelength Dispersion (WDXRF), with the objective of identifying rifle projectiles from different years of manufacture. For this purpose, ten samples of rifle projectiles, caliber 7.62mm, from the Companhia Brasileira de Cartuchos (CBC), with different years, were selected. The core of these projectiles were removed from the cartridge according to the procedure described by Dufosse and Touron2 and divided into three metal fragments that were later compacted in the form of 1 cm diameter discs and washed with 1% v / v HNO3, in an ultrasonic bath. The qualitative and quantitative analyzes of the samples were performed by WDXRF, using a Shimadzu® spectrometer (model XRF-1800). The spectral data obtained were treated using multivariate analysis, using the Unscrambler X® software. Chemometric analysis was able do correctly classify all projectiles according to their respective years of manufacture

Impressão digital metabólica para análise exploratória de plantas sob mudanças climáticas: estudo de caso de ecometabolômica

https://proceedings.science/p/120697

Ieda Spacino Scarminio [1]

[1] Universidade Estadual de Londrina

Improvements in the compositional analysis of sugarcane biomass

https://proceedings.science/p/120544

Paula Santana Barbosa [1]; Marcio Henrique Pereira Barbosa [2]; Bruno de Freitas Homem de Faria [3]; Reinaldo Teófilo [4]

[1] Química / UFV / Universidade federal de Viçosa; [2] Departamento de Agronomia / Universidade Federal de Viçosa; [3] Universidade Federal de Viçosa - Campus Florestal; [4] Universidade Federal de Viçosa

A specific procedure to chemical characterization of sugarcane bagasse is presented.
The removal of extractives and chromatographic analysis was optimized for sugarcane bagasse.

Isolation of mitraphylline from U. tomentosa barks and development of spectrophotometric method for alkaloids determination in cat´s claw samples

https://proceedings.science/p/120210

Marcos Martins Gouvêa [1]; Annibal Duarte Pereira Netto [1]; Samanta Mourão [1]; Flávia Ferreira de Carvalho Marques [1]

[1] Universidade Federal Fluminense

The alkaloid mitraphylline was efficiently obtained with small expense, and a simple and fast spectrophotometric method was suitable to determine total alkaloids in samples of Uncaria tomentosa.

LC-HRMS determination of glucose tetrasaccharide from urine samples collected on filter paper for diagnosis and monitoring of Pompe disease patients

https://proceedings.science/p/119965

Hygor Marcos Ribeiro de Souza [1]; Fernanda B. Scalco [2]; Flávia Ferreira de Carvalho Marques [1]; Rafael Garrett [2]
[1] Universidade Federal Fluminense; [2] Universidade Federal do Rio de Janeiro

Pompe disease is a lysosomal disorder in which acid α-glucosidase (GAA) enzyme deficiency lead to intralysosomal accumulation of glycogen in different muscle tissues.1 Although it is a rare disease (1:40.000 live births in the world) this anomaly has a significant impact, which can lead to death in the first years of life.2 One of the ways to diagnose the disease is by enzymatic/molecular analysis and urine glucose tetrasaccharide (T4) screening by HPLC.2 However, the use of these approaches are time-consuming or expensive and the shipping of urine samples is a critical factor. In this sense, we have developed and validated a methodology for determination of T4 in dried urine on filter paper (DUFP) using liquid chromatography-high resolution mass spectrometry (LC-HRMS). Then, this work has focused on 2 goals: (i) its applicability for screening, and (ii) to facilitate the collection and shipping of samples to reference centers as part of an early diagnostic investigation. Thus, control urine samples from health subjects were spiked with T4 standard solution, then mixed and added on 5 x 2.5 cm filter paper (Whatman 903). Then, it was dried for 24h on a plastic box at ambient temperature (22 °C ± 0.3). Finally, the extraction was performed using a mixture of ACN:H2O 1:1 %v/v containing 0.1% v/v of NH4OH under constant agitation for 15 min. The extract was centrifuged and analyzed by LC-HRMS. To the evaluation of metabolites stability the DUFP cards were stored at different temperatures: 4, 22 and 50 °C and times: 1, 3, 7, 15, and 30 days. LC-HRMS data were processed by the MS Dial software and the aligned data matrix (retention time + m/z) vs detected peak area were submitted to statistical analysis using GraphPad Prism software for one-way analysis of variance (ANOVA) test followed by Tukey post-tests and Metaboanalyst for PCA. As result, the developed method presented a linear range between 1 and 20 µg/mL, repeatability of 3.8% (n = 9), and the limit of quantification of 1 µg/mL demonstrated the high sensitivity of the method., Extracts fortified with T4 at three concentration levels, led to an overall mean recovery of 93 ± 3.8% (n = 9). T4 and other metabolites in DUFP were stable up to 7 days at 4 and 22 °C, and up to 3 days at 50 °C. Wang et. al. has showed that metabolic stability for liquid urine is just 24h at 4 and 22 °C.3 The method was applied to analyze urines from 15 Pompe patients and 15 healthy individuals collected on papers. The PCA model was applied and the results demonstrated that there is a trend of separation between control samples and Pompe samples in the space of two principal components that explain 73% of the variability. Therefore, the collection of urine on filter paper can be a viable alternative to avoid its rapid metabolic degradation. This demonstrates that proposed methodology was robust and the use of dried urine samples rises as possible alternative for collection material and facilitate in shipping urine without refrigeration. 1Muraoka, T. et.al.; Internal Medicine, 2011, 50, 2987. 2Chien, Y.H. e Hwu, W.L.; Biologics, 2007, 1, 195. 3Wang, X. et al. Metabolites, 2019, 9, 203.

Mapping of essentials elements on leaves of P. glomerata after grown with La2O3 nanoparticles using LA-ICP-MS technique

https://proceedings.science/p/120538

Vinicius Machado Neves [1]; Graciela Marini Heidrich [1]; Flávia Hanzel [1]; Cristian Pereira [1]; Fernando Nicoloso [1]; Valderi Luiz Dressler [1]
[1] Universidade Federal de Santa Maria

Elemental mapping in botanical tissue by LA-ICP-MS;
Effects of La2O3 nanoparticles on P. glomerata;
Distribution of essentials elements in P. glomerata leaves.

Microscale paper-based optoelectronic nose for identification of indoor air pollution caused by 3D printer thermoplastic filaments

https://proceedings.science/p/120408

Naira Souza Pinheiro [1]; Rafael Teixeira Freire [2]; Josiele Conrado [1]; Alex Domingues Batista [1]; João Flávio da Silveira Petruci [1]
[1] Universidade Federal de Uberlândia; [2] Barcelona Institute of Science and Technology

FDM 3D printers release over 200 toxic VOCs in 1 hour of printing; Our optoelectronic nose is able to detect the released compound and classify five different filaments within 20 min by HCA and PCA

Microwave-assisted ultraviolet digestion: an approach for the digestion of polymeric-based materials

https://proceedings.science/p/119871

Alice Penteado Holkem [1]; Leonardo Biluca de Oliveira [1]; Gabrielle Dineck Iop [1]; Erico Marlon de Moraes Flores [1]; Paola de Azevedo Mello [1]; Paola de Azevedo Mello [1]
[1] Universidade Federal de Santa Maria

Combination of microwave and UV radiation for improving sample preparation Decomposition of polymeric matrices using diluted acid solution Feasibility of halogens determination in acidic medium

Multivariate optimization of the anodic stripping voltammetry determination of metals in fuel bioethanol using disposable 3D-printed electrodes

https://proceedings.science/p/119541

Afonso Filipe João [1]; Sílvia Vaz F. Castro [1]; Raimundo R. Gamela [2]; Rafael Melo Cardoso [3]; Diego Pessoa Rocha ; Eduardo Mathias Richter [1]; Rodrigo A. A. Muñoz [1]
[1] Universidade Federal de Uberlândia; [2] Universidade Federal de São Carlos; [3] UFU

Box-Benheken design (BB) under response surface methodology (RSM was taken up to obtain the optimal conditions for relevant factors obtained in fractional factorial design (FFD);

Nanotubos de carbono magnético de acesso restrito para extração em fase sólida dispersiva de pesticidas organofosfatos em amostras de leite bovino

https://proceedings.science/p/120689

Ayla Campos do Lago [1]; Fabrício Alves Borges [1]; César Ricardo Teixeira Tarley [2]; Eduardo Costa Figueiredo [1]
[1] Universidade Federal de Alfenas; [2] Universidade Estadual de Londrina

The developed method exhibited suitable validation parameters, is simple, reproducible, quick, reduced the amounts of solvent consumed and promoted the exclusion of macromolecules

Nitrogen and phosphorus co-doped carbon dots: synthesis, characterisation and application in sensitive determination of Cr(VI) in water samples.

https://proceedings.science/p/119515

Josué Carinhanha Caldas Santos [1]
[1] Universidade Federal de Alagoas

Optimal conditions of amino acids extraction using carbon nanomaterial

https://proceedings.science/p/120480

Josimar Batista [1]; Helvécio Menezes [1]; Maria José Neves [2]; Zenilda Lourdes Cardeal [1]
[1] Departamento de Química / Universidade Federal de Minas Gerais; [2] Comissão Nacional de Energia Nuclear/ CDTN

BaP can change amino acid (AA) levels in yeast cell. AA can be biomarkers candidates. Carbon nanomaterial were applied to AA extraction. Desorption without heating was better to AA analysis by GC/MS.

Optimization and Validation of DLLME for the Simultaneous Determination of 2,3,7,8-TCDD and 2,3,7,8-TCDF in water samples

https://proceedings.science/p/120445

Lázaro Sicupira [1]; Gevany Paulino de Pinho [2]; Flaviano Silvério [2]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Universidade Federal de Minas Gerais

DLLME was used for the first time to determine 2,3,7,8-TCDD and 2,3,7,8-TCDF.
Easy and effective sample preparation methodology to determine 2,3,7,8-TCDD and 2,3,7,8-TCDF in water samples.

Optimization and validation of the LLE-LTP method for quantification of DDT in honey samples by HPLC-DAD

https://proceedings.science/p/120463

Lorena Maria Guimaraes Alves [1]; Lucas Victor de Freitas [2]; Lázaro Sicupira [1]; Flaviano Silvério [3]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] Faculdade de Ciências Farmacêuticas de Ribeirão Preto - Universidade de São Paulo - FCRP-USP; [3] Universidade Federal de Minas Gerais

LLE-LTP was applied to determine DDT in honey samples for the first time in this study.
The quantification limit reached met the Brazilian and European legislation.

Optimization of a DPX analytical method using Response Surface Methodology

https://proceedings.science/p/120309

Vanessa Alves [1]
[1] UFCat

O desenvolvimento de métodos analíticos capazes de determinar metais tóxicos é essencial, visto que a ocorrência desses íons metálicos nos diversos compartimentos ambientais tem sido cada vez maior. Diversas técnicas espectroscópicas são utilizadas para determina-los, porém nem sempre é possível, pois os mesmos podem estar presentes em concentrações inferiores aos limites de detecção do equipamento ou estarem presentes em uma matriz complexa, necessitando de etapas de extração e/ou pré-concentração. O método DPX pode ser utilizado para esse fim, o qual é baseado na SPE, consistindo de uma ponteira de micropipeta padrão “carregada” com o sorvente. Em métodos analíticos, diversas variáveis ou fatores podem influenciar seu desempenho, com isso, ferramentas quimiométricas multivariadas vêm sendo aplicadas. Nesse sentido, planejamentos experimentais podem ser utilizados, consistindo de um conjunto de experimentos definidos por uma matriz composta por diversas combinações de níveis das variáveis estudadas. O planejamento Doehlert vem se mostrando uma alternativa prática e econômica em relação a outros planejamentos (Planejamento de Composto Central e Box-Behnken), além de sua alta eficiência e a necessidade de poucos pontos experimentais para sua aplicação, são obtidas as condições ótimas (ponto crítico) através das características da superfície de resposta gerada. Assim, neste trabalho foram utilizados Planejamentos Doehlert para determinar os pontos críticos das variáveis que possivelmente mais influenciam o processo de adsorção (massa de adsorvente e número de ciclos) e dessorção (concentração do eluente e número de ciclos) de um método DPX em que se utiliza a Typha angustifolia L. como adsorvente para extração de íons Pb(II) e Mn(II), utilizando a detecção por FAAS. Ponteiras padrão de 5 mL tiveram suas extremidades inferiores vetadas com lã de vidro e preenchidas com material adsorvente nas quantidades de cada experimento. Nesse tipo de matriz, é utilizada uma equação para se determinar os valores experimentais, onde que para duas variáveis se tem um total de 7 experimentos, consistindo de um ponto central e mais seis pontos adicionais formando um hexágono regular. Para o processo de adsorção, o pH das soluções de ambos os íons foi ajustado para 8 e a concentração em 1,0 mg L-1 . Para o processo de dessorção, o eluente utilizado foi o HNO3 (ácido nítrico). As superfícies de resposta obtidas foram representadas por equações quadráticas, nas quais foi aplicado o critério de Lagrange e se identificou os valores críticos para cada otimização. Foram obtidos os pontos críticos de cada processo utilizando o software Statistica®. Para a etapa de adsorção foram identificados como sendo 31,32 e 28,81 mg de adsorvente para Pb(II) e Mn(II), respectivamente e 7 ciclos de adsorção para ambos os íons. Para a etapa de dessorção os valores encontrados foram de 0,8 mol L-1 para a concentração do eluente e 7 ciclos de dessorção. Com isso, o sistema de extração DPX foi completamente otimizado. O procedimento das isotermas de adsorção foi realizado no sistema DPX Os dados experimentais foram analisados graficamente, e avaliados frente aos modelos de Langmuir, Freundlich e SIPS. Ambos os íons, tiveram o melhor ajuste ao modelo de SIPS, indicando uma adsorção heterogênea. As capacidades máximas adsorvidas foram de 0,2942 mg g-1 e 0,5885 mg g-1 para Pb(II) e Mn(II), respectivamente. A utilização de metodologias de superfícies de resposta para a otimização de etapas em um

desenvolvimento de método analítico vem sendo cada vez mais difundida e consolidada, principalmente devido as suas vantagens em relação a otimização univariada, possibilitando uma resposta rápida e confiável, com menor tempo.

Otimização de um método analítico indicativo de estabilidade para estudar o perfil de degradação de uma formulação contendo anfotericina B

https://proceedings.science/p/120599

Thaís Bueno de Toledo [1]; Anderson Rodrigo Moraes de Oliveira [2]; Nayara C. P. de Albuquerque [1]; Franciane Marquele Oliveira [1]

[1] Eleve Science Pesquisa e Desenvolvimento; [2] Universidade de São Paulo

New formulation containing amphotericin B
Degradation profile study in formulations containing amphotericin B

Otimização e aplicação de método analítico para a determinação de resíduos de fármacos em amostras de águas superficiais

https://proceedings.science/p/120101

Tamires Santos Vaz [1]; Jeancarlo Pereira dos Anjos [2]; Pedro Afonso de P. Pereira [1]

[1] Universidade Federal da Bahia; [2] Centro Universitário SENAI CIMATEC

Os meios hídricos são receptores de esgotos domésticos, industriais e agropecuários e, consequentemente, são um importante veículo de dispersão ambiental dos poluentes químicos.[1] Apesar de sua função vital, os fármacos, quando presentes como contaminantes no ambiente, podem ser prejudiciais aos animais e seres humanos.[2] Eles se enquadram em um grupo de substâncias conhecidas como micropoluentes emergentes, sendo encontrados em matrizes ambientais e biológicas em concentrações muito baixas (ng L-1), mas potencialmente capazes de causar efeitos adversos em ecossistemas e/ou sobre a saúde humana.[3] O objetivo deste trabalho foi otimizar um método analítico, baseado em extração em fase sólida (SPE) e análise por HPLC-DAD, para a determinação de resíduos de sete fármacos em amostras reais de águas superficiais: cefalexina (CEF), cafeína (CAF), cloridrato de oxitetraciclina (OCT), tetraciclina (TC), sulfametoxazol (SMX), enrofloxacina (ENRO) e naproxeno (NPX). A separação dos fármacos foi realizada em coluna Poroshell 120 EC-C18 (100 x 2,1 mm, di = 2,7 mm) usando como fase móvel A: tampão 5 mM acetato de amônio/ácido acético B: acetonitrila/metanol (2:1, v/v), vazão de 0,2 mL min-1, utilizando um gradiente de eluição, com tempo total de corrida de 42 min. A extração dos analitos foi realizada utilizando SPE e foi otimizada por meio de planejamento experimental multivariado. Foram otimizadas as variáveis: volume de solvente para acondicionar o cartucho, pH e volume da amostra, espécie e volume do solvente para eluição e efeito salting out. O método exibiu resposta linear para os sete fármacos (R2 ≥ 0,9949), em faixas de concentração variando entre 10 e 500 µg L-1. Os limites de detecção e quantificação variaram de 7,4 a 18,1 µg L-1 e 24,7 a 60,4 µg L-1, respectivamente. A exatidão do método foi determinada a partir dos ensaios de recuperação, obtendo-se resultados que variaram entre 71,6% e 115% para os fármacos CEF, CAF, SMX, ENRO e NPX. No caso de OCT e TC, as recuperações variaram entre 28,8% e 70,3%, devido à possível degradação desses compostos. Estudos de estabilidade, executados durante um período de duas e vinte e quatro horas para os sete analitos, evidenciaram a rápida degradação para os fármacos OCT e TC. O método otimizado foi aplicado em amostra de água salgada (praia da Ribeira, em Salvador-BA, Brasil), de água doce (Rio Catu, município de Alagoinhas-BA, Brasil) e água de torneira (SENAI/CIMATEC, em Salvador-BA, Brasil). Na amostra de água salgada, foram encontrados os fármacos CEF, CAF e NPX, em concentrações de até 482 µg L-1; 37,6 µg L-1 e 40,3 µg L-1, respectivamente. Na amostra de água doce, foram encontrados os fármacos CEF, CAF, SMX, ENRO e NPX em concentrações de até 216 µg L-1; 3026 µg L-1; 290 µg L-1; 113 µg L-1 e 414 µg L-1, respectivamente. Na amostra de água de torneira, não foram encontrados fármacos. Verificou-se que, dos 5 fármacos determinados nas amostras, a cafeína apresentou uma alta concentração em água doce, o que pode ser explicado pelo seu uso generalizado pela população da região estudada (ex., consumo de bebidas cafeinadas). Além disso, as maiores concentrações encontradas nas amostras de água doce podem ser justificadas pela presença de atividades antrópicas no local, uma vez que o rio fica próximo à área urbana e industrial. O método otimizado, baseado em extração em fase sólida (SPE) e análise por HPLC-DAD, mostrou ser eficiente para a extração simultânea dos compostos-alvo nas amostras reais de águas superficiais.

Otimização e validação do método SLE/LTP para determinação de resíduos de agrotóxicos em farinha de trigo

https://proceedings.science/p/119514

Jéssika Faêda de Freitas [1]; Maria Eliana Lopes Ribeiro de Queiroz [1]; André Fernando de Oliveira [1]; Fernanda Fernandes Heleno [2]; Layssa Aparecida Abrantes [1]; Liany Divina Lima Miranda [1]

[1] Universidade Federal de Viçosa; [2] Serviço Autônomo de Água e Esgoto – Senador Firmino (MG)

O trigo se insere como matéria prima principal de diversos produtos alimentícios. Apesar de possuir alta produtividade, a cultura de trigo pode ser acometida por insetos-praga. Para a prevenção e controle de doenças agrícolas, normalmente são utilizados agrotóxicos, aplicados na fase de produção, na pós-colheita e no armazenamento, podendo levar à contaminação do produto final, caso seja usado de forma inadequada. Para avaliar a contaminação de farinha de trigo pelos agrotóxicos pirimifós-metílico, clorpirifós, tebuconazol, bifentrina, permetrina, cipermetrina e esfenvalerato, este trabalho teve como objetivo desenvolver o método extração sólido-líquido com partição em baixa temperatura (SLE/LTP), para determinar resíduos de agrotóxicos em farinha de trigo por cromatografia gasosa acoplada a espectrometria de massa (GC-MS). Na otimização multivariada do método foram avaliadas as variáveis volume de solvente extrator acetonitrila (ACN), volume de água destilada, tempos de agitação, de centrifugação e de congelamento. O método otimizado consistiu em acrescentar a 2,0000 g de farinha de trigo, 3,00 mL de água destilada, 4,00 mL de ACN em um frasco de vidro com capacidade de 22 mL. Essa mistura foi agitada em vórtex por 30 s, centrifugada por 3 min (1724 g) e refrigerada por 4 h em um freezer a -20 °C. Nessas condições as fases foram separadas e o extrato orgânico contendo os agrotóxicos analisado por GC-MS. O método otimizado foi validado, avaliando os seguintes parâmetros: seletividade, linearidade, limites de detecção e quantificação, exatidão e precisão. Os limites de detecção foram entre 0,23 a 6,6 µg kg-1 e os limites de quantificação entre 0,68 a 19,7 µg kg-1, valores considerados abaixo dos limites máximo de resíduos permitidos (LMRs). Os valores de recuperação ficaram no intervalo de 86,1 e 115,8%, com precisão ≤ 20%. O método SLE/LTP desenvolvido, otimizado e validado foi aplicado na determinação de agrotóxicos em amostras de farinha de trigo adquiridas em supermercados e feiras de Viçosa-MG, a fim de verificar a eficiência do método proposto. Todas as amostras apresentaram resíduos de pelo menos um dos agrotóxicos avaliados neste trabalho. Assim, todos os agrotóxicos determinados nas diversas amostras de farinha de trigo, farinha de trigo integral e farelo de trigo apresentaram valores iguais ou acima do LMR permitido pela União Europeia (EU), exceto a cipermetrina. Já pela ANVISA, duas amostras tiveram o nível de resíduos dos agrotóxicos permetrina e tebuconazol acima do LMR. O pirimifós-metílico foi determinado na maioria das amostras com concentrações entre 0,02 a 0,51 mg kg-1, sendo que esse é o agrotóxico mais utilizado em cereais. Esses resultados mostram a necessidade de se continuar monitorando a presença de resíduos nesta matriz. Conclui-se que o método desenvolvido resultou em um método viável para análise dos analitos em amostras de farinha de trigo, por ser simples, eficaz, com baixo consumo de solvente e a extração realizado em etapa única.

Otimização multivariada aplicando modelo Doehlert de três variáveis para síntese de biocombustível utilizando óleo residual, metanol e catalisador alcalino

https://proceedings.science/p/120552

Breno Assunção Brito [1]; Victor Hugo Simões Borges [2]; Felipe Cairo Menezes [3]; Ingridy Santos Lopes [3]; Camila Lopes [1]; Simone Chiapetta [2]

[1] Instituto Nacional de Tecnologia - INT; [2] Instituto Nacional de Tecnologia; [3] Outros

The Doehlert Methodology was used as a tool to study the transesterification reaction of residual oils to obtain methyl esters for use as biofuel.

Potentiality of electrochemical methods of analysis for on-site applications

https://proceedings.science/p/122103

Eduardo Mathias Richter [1];

[1] Universidade Federal de Uberlândia

Nesta apresentação, a potencialidade de métodos eletroquímicos de análise para uso em campo será discutida (portabilidade). O objetivo é mostrar uma visão crítica em relação a aspectos relacionados a robustez, praticidade e frequência analítica deste tipo de método de análise. Experiências de nosso grupo de pesquisa nesta área serão abordados.

Prediction of Sucrose using Near-Infrared Spectroscopy of Dehydrated Sugarcane Juice and PLS Models

https://proceedings.science/p/120535

Wilson Cardoso [1]; João Gabriel Gomes Rangel [2]; Marcio Henrique Pereira Barbosa [3]; Reinaldo Teófilo [2]
[1] Universidade Federal de Viçosa; [2] Department of Chemistry, Universidade Federal de Viçosa; [3] Departamento de Agronomia / Universidade Federal de Viçosa

A dehydration method was used to remove water and concentrate the sample.
OPS method was used to select the most predictive variables.

Preparation of magnetic MIP for extraction/ preconcentration of tetracyclines in food samples and determination by HPLC-DAD

https://proceedings.science/p/120434

Luciane Effting [1]; Caroline Teixeira Lopes [1]; Milena do Prado Ferreira [1]; Suzana Lucy Nixdorf [1]; César R. T. Tarley [2]
[1] Universidade Estadual de Londrina; [2] Universidade Estadual de Campinas

Tetracyclines used in veterinary treatments due to their antimicrobial action. Semi-covalent imprinting approach in magnetic surface for tetracycline adsorption. Magnetic molecularly imprinted polymer

Preparo de amostras usando ácido fórmico diluído para determinação elementar em crustáceos por MIP OES

https://proceedings.science/p/120630

Michelle de Souza Lemos [1]; Kelly G. Fernandes Dantas [2]
[1] Instituto de Ciências Exatas e Naturais / Universidade Federal do Pará; [2] Universidade Federal do Pará

Sample preparation was performed using diluted formic acid
The determination of Al, Cr, K, Mg, Mn and Zn was performed by MIP OES.
The procedure was adequate for the determination of analytes

Procedimento alternativo para decomposição de amostras com alto teor de sílica

https://proceedings.science/p/120569

Rafael Mantovaneli [1]; Matheus Barbosa Rasch [1]; Bruna Dalfior [1]; Geisamanda Pedrini Brandão [1]; Joaquim Araújo Nóbrega [2]; Maria Tereza Carneiro [3]
[1] Universidade Federal do Espírito Santo; [2] Universidade Federal de São Carlos; [3] UFES

Use of HBF4 in the preparation of high silica samples. Factorial mixtures design for optimization for sample preparation. Trace elements determination by atomic spectrometry.

PRODUÇÃO DE CARVÃO ATIVADO A PARTIR DA CASCA DE SEMENTES DE PINHÃO (Araucária angustifolia)

https://proceedings.science/p/120016

Elizabeth M. Nebes [1]; Alessandra Stevanato [1]; Delia do C. Vieira [2]; Roger N. Michels [3]; Janksyn Bertozzi [1]
[1] Departamento Acadêmico de Química, UTFPR - Londrina; [2] Departamento Acadêmico de Engenharia de Materiais, UTFPR - Londrina; [3] Departamento Acadêmico de Engenharia Mecânica, UTFPR - Londrina

Production of activated charcoal from the pine seed peel (Araucária angustifólia).
Optimize the process of production of activated carbon
Central rotational composite planning

Pyrolysis–GC–MS of asphaltenes for the hydrocarbon screening in highly biodegraded crude oils

https://proceedings.science/p/120685

Bruno Quirino Araújo [1]; Bruno Fioresi Paqueli [1]; Marcos Henrique Oliveira Petroni [1]; Madson Poltronieri Zanoni [1]; Geraldo Ferreira David [1]; Cristina Maria dos Santos Sad [1]; Sergio Antonio Fernandes [2]; Valdemar Lacerda Jr. [1]

[1] Universidade Federal do Espírito Santo; [2] Universidade Federal de Viçosa

Geochemical investigation of occluded and chemically bonded hydrocarbons of asphaltenes. Evaluation of asphaltenes from highly biodegraded crude oils (Espírito Santo Basin) using pyrolysis–GC–MS.

Química analítica verde aplicada em amostras de alimentos

https://proceedings.science/p/120698

Wanessa Melchert Mattos [1]

[1] Universidade de São Paulo

Restricted access carbon nanotubes for microextraction by packed sorbent to determine antipsychotics in plasma samples by UPLC-MS/MS

https://proceedings.science/p/120457

Jonas Carneiro Cruz [1]; Maria Eugenia Queiroz Nassur [1]; Eduardo Costa Figueiredo [2]; Henrique Dipe de Faria [2]

[1] Universidade de São Paulo; [2] Universidade Federal de Alfenas

The method was successfully applied for TDM of antipsychotics in untreated plasma samples. The RACNTs were successfully applied as MEPS sorbent excluding about 97% of the plasma proteins

Salting-out Induced Liquid-Liquid Microextraction - SILLME: a green technique for the determination of preservatives in processed food samples

https://proceedings.science/p/120208

Jean Lucas de Oliveira Arias [1]; Caroline Borges Rocha [1]; Larine Kupski [2]; Sergiane Sousa Caldas [1]; Ednei Gilberto Primel [3]

[1] Universidade Federal do Rio Grande - FURG; [2] Universidade Estadual de Maringá - UEM; [3] Universidade Federal do Rio Grande-FURG

Among the different preservatives allowed for use in foods, benzoates, sorbates and parabens can be highlighted. These preservatives act as antimicrobial agents, protecting food against contamination by molds, yeasts and bacteria (ESIMBEKOVA et al., 2017). Once these substances are strange to our body, being potentially toxic, it is necessary to control the exposition, as well as establishing safe limits for their usage. The evaluation of safety in use of preservatives is based on the control of the Acceptable Daily Intake (ADI), which means the amount of substances that can be ingested daily without risks to health, even in long exposure. For such purpose, the continuous evaluation of these levels in different foods is necessary. In this work, a method for the determination of preservatives in processed foods from different categories, such as dairy products, non-alcoholic beverages, spices and sauces, fruit jams and pastes, preserves and artificial sweeteners was optimized. The method deal with extraction by Salting-out Induced Liquid-Liquid Microextraction (SILLME) with determination by High Performance Liquid Chromatography with Ultraviolet Detector (HPLC-UV). After the evaluation of MgSO4 amount, sample pH and the addition of NaCl, the method was performed as follows: 1 g sample was weighed in a 15 mL polypropylene tube and acetate buffer pH 4.2 was added up to 5 mL. Then, 1 mL acetonitrile was added to the mixture, which was vortexed for 1 min.After, 2 g MgSO4 were added to the mixture, which was agitated again, followed by centrifugation for 5 min at 7793 x g; finally, 500 µL of the acetonitrile layer was collected and diluted up to 1 mL with ultrapure water in a HPLC vial. Experiments were performed in triplicate. The method proved to be accurate, with recoveries between 80 and 103%, and precise, with relative standard deviation ≤ 11% and measurement uncertainty ≤ 31%. The method limits of quantification were between 0.03 and 0.07 mg kg-1, being adequate for the determination of these preservatives in processed food samples. SILLME method was applied successfully in the determination of preservatives in processed foods, being determined concentrations up to 814 mg kg-1 for benzoate, 1154 mg kg-1 for sorbate and 461 mg kg-1 for methylparaben. Additionally, this method was compared to a previously optimized QuEChERS method developed by

our group (ARIAS et al., 2019), where data agreement between 94 to 99% was achieved. Finally, an efficient and simple method was developed that can be used in replacement of the traditional ones in routinely determination of preservatives in different kind of foods, with the advantages of being simpler, faster and cheaper than the official methods. ARIAS, J. L. O. et al. Fast and simple method of simultaneous preservative determination in different processed foods by QuEChERS and HPLC-UV: Method development, survey and estimate of daily intake. Food Chemistry, v. 293, p. 112-119, 2019. ESIMBEKOVA, E. N. et al. Inhibition effect of food preservatives on endoproteinases. Food Chemistry, v. 235, p. 294-297, 2017.

Selective determination of pesticides by synchronized scanning fluorescence and photochemical derivatization

https://proceedings.science/p/120278

Rosana Candida Macedo [1]; Vanessa dos Santos Oliveira [1]; Alice Cabral Paredes [1]; Matheus Delduque S. da Silva [1]; Joseany M. S. Almeida [2]; Ricardo Aucélio Queiroz [2]; Alessandra Licursi Maia Cerqueira da Cunha [1]
[1] IFRJ; [2] PUC

The presence of pesticide residues in agricultural products raises serious environmental and health concerns. The development of simple, sensitive and selective analytical methodologies is crucial to monitor the use of these substances. Early fluorometric assays investigated the possibility of quantifying some strobilurins (important fungicide class) using photoderivatization as a tool for the fluorimetric determination. Photoderivatization was applied to induce the formation of products with a more rigid molecular structure, thus with higher fluorescent quantum efficiency with less residue generation. Better results were obtained for kresoxim-methyl (KRESO) with gain of 2820% after UV exposure and trifloxystrobin (TRIF) with gain of 791%. The flexibility and sensitivity of spectral techniques arise from the fact that waveforms can be used to select different classes of chromophores. In this sense, fluorescence is a promising tool capable of detecting small differences between similar substances or materials. Presenting more selectivity than the emission and fluorescence excitation techniques, the synchronized scanning fluorescence (where both excitation and emission monochromators are scanned simultaneously) discriminates against small differences by means of the specific Δl of the analyte to be determined. In this work, it was associated synchronized scanning fluorescence as instrumental tool for the selective determination of these fungicides in the presence of possible interferents (in this case, triazoles presents in commercial formulations). Solutions of KRESO (30.0 µg mL-1) and TRIF (40.0 µg mL-1), using acetonitrile/ultrapure water (50/50% v/v for KRESO and 70/30% for TRIF), were prepared separately and combined with triazoles (tebuconazole, TEB or cyproconazole, CIP). Afterwards, the solutions were exposed to UV radiation for 15s (reactor of own manufacture - LEEA PUC-Rio). The measurements were made by spectrofluorimetry Perkin Elmer LS45 at Δλ = 64 nm (λexc/em = 373/437 nm) and Δλ = 36 nm (λexc/em = 338/374 nm) for KRESO and TRIF, respectively. In Table 1 are presented the sample compositions and the ratio between the fluorescent signal intensities of the mixture (analyte + interferent) by analyte solution. The analytical response of these substances in function of the measured signal presented promising results (LOD 9.7 ng mL-1 and CV(n=5) < 5% for KRESO and LOD 58.0 ng mL-1 and CV(n=5) < 3% for TRIF). As according to European (EU 2016/486) and the Brazilian (SINITOX/ICICT/FIOCRUZ, 2015) legislations, the LODs are below the required specifications. Based on these results, the synchronized scanning fluorescence can be considerate a simple and selective tool for the determination of KRESO and TRIF. Applicability in complex samples are still in progress. Table 1: Sample compositions and ratio between the fluorescent signal intensities of the mixture (Ianalyte + interferent) by analyte solution (Ianalyte). Sample Composition Ianalyte+interferent / Ianalyte TRIF + CIP (2:1 m/m) 1,00 TRIF + TEB (1:2 m/m) 1,01 KRESO + TEB (1:1.25 m/m) 0,98

Sorption of triazines from water using polyurethane foams (PU) as sorbents

https://proceedings.science/p/120489

Luis Fernando Amorim Batista [1]; Sara Renata Gonçalves [1]; Sônia Faria Zawadzki [1]; Gilberto Abate [1]
[1] Universidade Federal do Paraná

The synthesis of PU was made by using a complete 2^4 factorial planning. Some PU sorbed near 100% of all analytes. PEG 400 used in synthesis step showed an important role in the sorption of triazines.

SpectroscoPi: Exploring the advantages of 3D printing in the development of spectroscopy instrumentation

https://proceedings.science/p/120444

Ítalo Caliari [1]; José Vitor Nicacio [2]; Marcio Henrique Pereira Barbosa [3]; Reinaldo Teófilo [1]

[1] Departamento de Química / Universidade Federal de Viçosa; [2] Departamento de Engenharia Agrícola / Universidade Federal de Viçosa; [3] Departamento de Agronomia / Universidade Federal de Viçosa

A 3D printed near infrared spectrometer (800-1600 nm) was built. No optical alignment and wavelength calibration were made. The spectrometer shown promisors qualitative and quantitative results.

Spot test using digital image for determination of propoxur based in indophenol blue formation

https://proceedings.science/p/119562

Karoline Rayzel [1]; Wanessa Melchert Mattos [1]

[1] Universidade de São Paulo

Development of a fast, practical and cheap analytical method for determination of propoxur based on spot test and digital image.

Ultrasensitive microfluidic immunosensor based on electrodeposited nanoporous gold for cancer biomarker detection

https://proceedings.science/p/119781

Daniel Matias Gaston Regiart [1]; Mailen G. Neira [2]; Alba Marina Gimenez [3]; Marcelo N.P. Carreño [4]; Mauro Bertotti [1]

[1] Instituto de Quimica - USP; [2] UNSL; [3] School of Pharmaceutical Sciences - USP; [4] Escola Politécnica

SOX-2, a protein also known as SRY-box 2 (Sex determining Region Y-box 2), is a transcription factor whose function is essential in the regulation of embryonic development, the induction of mother cell pluripotentiality, and the determination of cell differentiation [1]. Several mutations in this gene have been associated with a severe malformation in the eye structure called anophthalmia. It has also been determined that the ectopic expression of SOX-2 could be related to abnormal differentiation of colorectal cancer cells, as well as to overexpression in breast, ovarian, lung, esophageal, prostate, pancreatic, testicular, and cutaneous, neck and head squamous cell carcinoma, among others [2]. We developed an ultrasensitive and portable microfluidic electrochemical immunosensor for SOX-2 determination in human serum samples. The selectivity and sensitivity of the sensor were improved by using a hybrid PDMS-glass microfluidic channels modification based on a physical-chemical treatment to obtain a hydrophilicity functional platform, with an increased surface to volume/ratio, where the anti-SOX-2 antibodies can be covalently immobilized. The characterization of the modified channel surface was carried out by Infrared Spectroscopy. Moreover, the gold electrode surface was modified by using a dynamic hydrogen bubble template, and a gold nanoporous structure (NPAu) was obtained. Such platform has outstanding properties, like high specific surface area, large pore volume, uniform nanostructure, good conductivity, and excellent electrochemical activity [3]. NPAu was characterized by scanning electron microscopy, energy dispersive spectrometry, cyclic voltammetry, and X-ray diffraction. SOX-2 present in the samples binds to the anti-SOX-2 immobilized and was then quantified by using a second antibody labeled with horseradish peroxidase (HRP- anti-SOX-2). Finally, a H2O2 + 4-tert-butyl catechol solution was added, and the enzymatic product (quinone) was reduced on the NPAu electrode at +100 mV (vs. Ag). The current obtained is directly proportional to the SOX-2 concentration in the sample. The detection limit was found to be 30 pg mL-1, and the coefficient of variation was less than 3.75 %. As it can be seen, the microfluidic electrochemical immunosensor is a suitable clinical device for in situ SOX-2 determination in real samples.

Use of digital images and smartphone to determine soluble proteins in Whey protein using the Bradford method

https://proceedings.science/p/119992

Bruna Soares Dionizio [1]; Daiane Daniel [1]; Diego Victor de Babos [1]; Edenir Rodrigues Pereira-Filho [1]; Dulce Helena Ferreira de Souza [1]

[1] UFSCar

Currently, there has been an increase in the consumption of sports supplements such as whey protein, consisting of proteins derived from milk, by practitioners of physical activity, with the aim of increasing the synthesis of muscle proteins1. One of the colorimetric methods used to determine total proteins is the Bradford method using UV-Vis spectrophotometer2. The use of digital devices such as cameras and smartphones and PhotoMetrix® software has been employed to perform colorimetric detection, aiming at the speed, practicality and low cost of analysis when compared to the spectrophotometer3. Thus, a study was developed in order to determine the total soluble proteins in 9 samples of sports supplements using digital images and PhotoMetrix®. To prepare the sample, 100 mg of each sample was solubilized in 10 mL of ultra-pure water and centrifuged. The calibration curve was prepared with 0 to 0.8 mg mL-1 of bovine serum albumin (BSA) protein. An aliquot of 20 µL of each sample was added to 1000 µL of Bradford's solution and homogenized. After 5 minutes of incubation (25 °C), the absorbance can be read at 595 nm using a spectrophotometer (reference method), as well as digital images were acquired with a 13 MP camera from a Samsung J500-M cell phone, then processed by the PhotoMetrix®. Addition-recovery experiments were performed with 3 samples, adding 1 mg mL-1 of BSA, to assess the accuracy of the method. To analyze the protein profile, supplement samples were submitted to gel electrophoresis. The analytical performance parameters obtained with the reference method were limits of detection (LOD) and quantification (LOQ) of 0.003 mg mL-1 and 0.01 mg mL-1, respectively of total soluble proteins, and RSD values in the range of 1-11%. When using PhotoMetrix® for protein quantification, the LOD and LOQ obtained were 0.0002 mg mL-1 and 0.0007 mg mL-1, respectively. The method demonstrated good precision of the measurements with RSD in the range of 1-13%. The addition and recovery experiments demonstrated good accuracy for both methods, with recoveries of 82-112% using PhotoMetrix®, and 84-106% using the reference method. It was observed that the LOD and LOQ values determined by PhotoMetrix® were 15-fold lower than the values obtained by the reference method. The concentrations of total soluble proteins (n = 3), determined in the 9 samples of commercial sports supplements ranged from 17±1 to 253±12 g kg-1 using the reference method, while PhotoMetrix® presented results between 14±1 to 304±33 g kg-1, demonstrating that the values determined by both strategies are in concordance. Besides that the formulations present great variability of concentration of total proteins solutions. Through the electrophoretic gel it was possible to observe that the sample #1 (S1) differs from the other samples qualitatively, and this result corroborates with the determined concentrations: this samples presented the lowest protein in its formulation. Thus the proposed procedure using PhotoMetrix® proved to be an excellent analytical tool for the determination of low concentrations of soluble proteins using the Bradford method. [1] F.K. Haraguchi et al., Rev. Nutr., 19(4) (2006) 479-488. [2] M.M. Bradford, Anal. Biochem., 72 (1976) 248. [3] PhotoMetrix Database: http://www.photometrix.com.br.

Use of factorial design for optimization of microwave-assisted digestion of maize flour using ICP-OES technique

https://proceedings.science/p/120636

Danylo David de Lima Silva [1]; Maria José de Filgueiras Gomes [1]; Gabrielly Simões Ferreira [1]
[1] Universidade Federal Rural de Pernambuco

Maize flour mass of 400 mg was digested with only 4 mL of 14 mol L-1 HNO3, 2 mL of H2O2 (30%), 1 mL of H2O and temperature of 160 °C; Residual carbon content was quantified in samples using ICP-OES.

Using untargeted Metabolomics to understand the mode of action of drugs and bioactive compounds against Leishmania parasites

https://proceedings.science/p/119847

Gisele André Baptista Canuto [1]
[1] Universidade Federal da Bahia

Metabolomics is a powerful tool to understand biological systems. Analytical multiplatforms provide a broad coverage of the metabolome.

Uso da técnica de microextração por sorvente empacotado (MEPS) na extração e pré-concentração de agrotóxicos em água.

https://proceedings.science/p/120453

Wagner Aires de Oliveira Júnior [1]; Silvia de Sousa Freitas [1]
[1] Universidade Federal de Catalão

Use of microextraction by packed sorbent (MEPS) tecnique for extraction and pre-concentration of pesticides in water. Iprodione and tebuconazole were pre-concentrated 18.2 and 21.5 times, respectively, by the MEPS procedure proposed.

Validação Analítica por HPLC-DAD para Determinação de Estrogênios em Águas

https://proceedings.science/p/120790

Ana Rosa da Silva Neta [1]; José Licarion Pinto Segundo Neto [2]; Gilvan Pozzobon Pires [1]; Mário Ugulino de Araújo [3]; Kátia Messias Bichinho [3]
[1] PPGQ/Universidade Federal da Paraíba; [2] Departamento de Química Fundamental/Universidade Federal de Pernambuco; [3] Departamento de Química/Universidade Federal da Paraíba

Emerging contaminants are unregulated substances.
Endocrine disruptors are harmful to the aquatic ecosystem and human health.
Reliable methods are needed to determine emerging contaminants.

Validation of a bioanalytical method for further pharmacokinetic studies of amphotericin B in an innovative formulation

https://proceedings.science/p/119955

Maraine Catarina Tadini [1]; Icaro Salgado Perovani [2]; Franciane Marquele-Oliveira [1]; Anderson Rodrigo Moraes de Oliveira [3]
[1] Eleve Science Pesquisa e Desenvolvimento; [2] Departamento de Química / Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto / Universidade de São Paulo; [3] Universidade de São Paulo

Development of more safety formulation with AmB
Validation of a bioanalytical method to analyze AmB in rat plasma
All parameters agreed with ANVISA guidelines

Química Biológica - BIO

Analysis of cysteine peptidase gene expression during insect developmental stages by RT-qPCR

https://proceedings.science/p/119508

Katia Celina Santos Corrêa [1]; Kelli Micocci [1]; Dulce Helena Ferreira de Souza [1]
[1] Universidade Federal de São Carlos

Analysis of cysteine peptidase gene expression during insect developmental stages by RT-qPCR Leaf-cutting ants are considered the most important herbivorous insects, commonly depending on fresh plant leaves, which serve as substrate for symbiotic fungus culture1. These insects are known for their high damage power to agriculture and natural forests or reforestation. In insect cysteine peptidases have been expressed on stage of development in several organisms, such enzymes have been identified in metamorphosis and tissue reconstruction2, which suggesting these enzymes have a great potential to be used as molecular targets to developing new insecticides. Previously studies in our laboratory, the DNA of a cysteine peptidase of Atta Sexdens ants was cloned, and recombinant enzyme was expressed in E.coli, purified and tested against cysteine peptidase inhibitors. To understanding the role of the enzyme

in these organisms, trying to infer which metabolic pathway is involved, the aim of this present work was analyzed the gene expression quantitatively by RT-qPCR in the different stages of A. sexdens life (pupae, larvae and worker) and in some parts of the worker body (head, mesosoma, gaster and the body without gaster (WWG). The cDNA from insect developmental stages and its body parts were used as a template for independent qPCR reactions. RT-qPCR was performed using the StepOneTM Real-Time PCR System (Thermo Fisher Scientific) with total volume reaction of 12 µL: 6 µl of Power SYBR® Green PCR Master Mix (Thermo Fisher Scientific), 3 µl (about 1.7 ng) of diluted cDNA and 3 µl of mix solution containing forward and reverse primers (according with the F/R relation). Thermal cycling conditions for all genes were: 15 minutes at 95 °C, followed by 40 cycles of 95 °C for 15 seconds, 60 °C for 60 seconds and 95 °C for 15 seconds. An analysis of relative gene expression data was calculated using the 2−ΔΔCt method as described 3 The statistical analyses were performed with GraphPad Prism 5 software. The mean comparisons were computed by analysis of variance (ANOVA). Tukey's multiple comparisons tests were used for post hoc analysis. $P < 0.01$ (**) and $p < 0.001$ (***) were considered statistically significant. The gene was expressed throughout the life cycle of the insect which suggests a more general role for the enzyme, as well as the lysosomal function. Among the body parts of adult , there is no difference in the expression pattern gene transcription and the results showed that the gaster represent a significative importance in the cysteine peptidase transcript expression.

Are the illicit drugs 25H-NBOH and 25H-NBOMe toxic to zebrafish embryos?

https://proceedings.science/p/119468

Wellington Alves de Barros [1]; Juliana Alves da Costa Ribeiro [2]; Leonardo Rogério Vieira [2]; Marcelo Pereira Queiroz Pereira [1]; Graziele Martins Borges [1]; Davi Felipe Farias [2]; Ângelo de Fátima [3]

[1] Universidade Federal de Minas Gerais; [2] Universidade Federal da Paraíba; [3] Universidade Federal de Minas Gerais

Substances named as NBOH and NBOMe comprise a family of phenethylamines that act as serotonin receptor agonists (5-HT2 family), causing hallucinogenic effects. These substances have been sold as recreational drugs and several deaths have been reported after the ingestion of these phenethylamines; however, there are no studies evaluating their in vivo toxic effects. Zebrafish (*Danio rerio*) is a tropical teleost fish which is a recognized animal model in biomedical research due to the low-cost maintenance, high fecundity, short life cycle, and high similarity of its genome to the human genome. These advantages confer *D. rerio* a useful model for application high performance techniques for screening new drugs and their potential toxic effects. In this work, we have studied the effects of illicit drugs 25HNBOH and 25H-NBOMe *in vivo* using zebrafish embryos. The embryos with up to 3 hours post fertilization of age were exposed to five crescent concentrations of 25H-NBOH (5, 10, 20, 40 and 80 mg/L) and 25H-NBOMe (5, 20, 50, 70 and 100 mg/L) for 96 h and the apical endpoints were analyzed each 24 h post-incubation to the drugs. The number of deaths was used to calculate the LC50. Additionally, sublethal effects were also recorded daily. Observations were performed in a stereomicroscope (x 80 magnification) and photographed (Zeiss). The activities of cholinesterase (ChE), lactate dehydrogenase (LDH) and glutathione S-transferase (GST) were determined for both substances in embryos exposed to three concentrations below the LC50. At the highest concentrations tested (80 and 100 mg/L of 25H-NBOH and 25H-NBOMe, respectively), both samples caused high embryo mortality and coagulation was the only endpoint for lethality observed. By decreasing the concentration of the tested-substances, lethality also decreased while non-lethal effects were predominant up to 10 and 50 mg/L of 25H-NBOH and 25H-NBOMe, respectively. The non-lethal effects observed were spine malformation, egg hatching delay and body malformation for both drugs, while otolith malformation, pericardial edema and blood clotting were found only for 25H-NBOMe. 25H-NBOH and 25HNBOMe showed distinct toxicity profiles to zebrafish embryos, the LC50 values showed that 25H-NBOH was more lethal (LC50 43.38 mg/L) than 25H-NBOMe (LC50 82.96 mg/L). The activities of the enzymes ChE, LDH and GST were changed by 25H-NBOH and 25H-NBOMe, indicating that their toxic properties could be associated with the negative effects of these drugs on such enzymes. The quantification of the biomarker's activities showed that 25H-NBOH has significantly changed the activity of the three enzymes, but the ChE activity was the most affected. Our results showed that 25H-NBOH and/or 25H-NBOMe possess in vivo (neuro)toxic effects to zebrafish embryos and their sublethal effects, most accounting for teratogenicity, were quite relevant in lower concentrations. Highlights -Toxic effects of 25H-NBOH and 25H-NBOMe on zebrafish embryos were evaluated. -Both substances were teratogenic to zebrafish embryos and negatively modulated the activities of ChE, LDH and GST

Capacitive electrical stimuli applied to differentiation process from human Mesenchymal Stem Cell to bone cell over PEDOT-co-PDLLA.

https://proceedings.science/p/120280

Rubens Araujo da Silva [1]
[1] Instituto de Química - USP

Damage caused by thimerosal linked to human erythrocyte hemoglobin: mechanism of action up to structural changes.

https://proceedings.science/p/119551

Marcos Vinicius dos Santos Sales [1]; Reginaldo C. da Silva Filho [2]; Marina M. Silva [2]; ISIS FIGUEIREDO [2]; Carlos Jacinto [2]; Ueslen Rocha [2]; Josué Carinhanha Caldas Santos [2]; Ana Catarina R Leite [2]
[1] Universidade Federal de Alagoas ; [2] Universidade Federal de Alagoas

INTRODUCTION: Thimerosal (TH) is a mercury-based organic compound used as a preservative in many vaccines. When, in the human body, it is metabolized or degraded to ethylmercury and thiosalicylate. The ethylmercury has a high affinity to thiol functions of proteins and can, therefore, bind to protein matrices like human hemoglobin because of its several free thiol functions [1]. Also, this structure can interact with human erythrocytes (Ery) affecting the O2 uptake by hemoglobin. In this context, this work evaluated the interaction of thimerosal with human hemoglobin (HbTH) through monitoring its ability to reduce the binding capacity of Hb toward O2. In these measures, Ery, from adult humans, have been exposed for two different concentration of TH (1.25 and 2.50 μM) with an incubation time of 3 min (or 5 min) for two temperatures 28 and 37°C. MATERIAL AND METHODS: Ery were used to evaluate O2 uptake, considering the following variables: TM concentration (1.25 and 2.50 μM), incubation time (3 or 5 min) and temperature (28 and 37°C), we also tested HgCl2 as a positive control. Sulfidryl content and Raman spectrum changes in the presence of TM were also evaluated. RESULTS AND DISCUSSION: In assays the time of 5 min showed the most pronounced responses in Ery, as the reduction of O2 uptake at 28°C, that was 38% (1.25 μM) and 51% (2.50 μM). At 37°C it reached 51% (1.25 μM) and 61% (2.50 μM). Mercury chloride, used as a control, showed at least 62% of reduction in O2 uptake. The -SH assays quantified the preservation of these groups up to 59% at Ery in the presence of NEM (reducing agent). In the Raman spectrum we verified differences in regions that are related to Fe-O bond and distortion of the hemoglobin porphyrinic ring. CONCLUSION: Based on our results, it is suggested that TM binds to hemoglobin causing conformational changes and these leads to a deleterious effect on its primary O2 binding function.

Effect of native and non-native metals on human co-chaperone Hsp40 investigated by metallomic study using LC-ICP-MS and ITC

https://proceedings.science/p/119929

Jemmyson Jesus [1]; Marco Aurélio Zezzi Arruda [1]; Carlos Henrique Inacio Ramos [1]
[1] Unicamp

There is evidence that the homeostasis of metals has an important medicinal role since the disturbance of the equilibrium appears to be related to several diseases and to aging. Actually, the dietary supplementation of zinc, and to a lesser extent copper, seem to alleviate the symptoms of neurodegenerative diseases and dementia. Curiously, there is also mounting evidence that molecular chaperones and heat shock proteins (Hsps) participate in metal homeostasis, since their expression increases when metals are added to the cellular environment. DNAJA1 is a class A J-protein (Hsp40) from a human that has two zinc finger domains within its structure and plays a crucial role in maintaining cell proteostasis. A recent study from our group showed that Zn2+ plays an important role in the stability and functional activity of YdJ1 (a class A J-protein (Hsp40) from yeast)*. Specifically, it was observed that Znremoval decreases both the stability and chaperone activity of Ydj1. Thus, a new question arises: Could a metallochaperone incorporate a non-native metal cofactor within its structure and maintain its thermal stability and functional activity? This work presents a thermodynamic study of the interaction between DNAJA1 and four essential metal ions (Zn2+, Cu2+, Fe2+, Mg2+), as well as a kinetic study of the functional activity after incorporation of these metal ions. Recombinant DNAJA1 was produced and purified and a method optimized by Jesus et al.1 was applied for Zn-removal and LC-ICP-MS analysis was applied to check the presence of metals (Zn, Fe, Cu, and Mg). ITC was applied to obtain the thermodynamic data of the interaction and CD was used to investigate both the secondary structure and thermal stability of the protein. In addition, chaperone activity was studied by measuring the ability of DNAJA1 to prevent luciferase aggregation before and after Zn-removal, as well as after incorporation of other metals. The results are as follows. DNAJA1was ~95%

pure and had both significant Zn-removal after application of the method and significant incorporation of the metal ions as showed by ICP-MS analysis. ITC showed that binding reactions were exothermic and chaperone activity measurements are underway Reference: *Jesus et al. Frontier in Chemistry. V. 7 (2019) p1-10

Identification and purification of a lectin from leaves of Jatropha multifida L. (Malpighiales: Euphorbiaceae)

https://proceedings.science/p/119582

Anyelly Gomes Santos [1]; Camila Pereira de Lima Chicuta [1]; Andrea Carla de Almeida Barros [1]; Francis Soares Gomes [1]
[1] Universidade Federal de Alagoas (UFAL)

Jatropha multifida is used in folk medicine as a healer for the treatment of oral thrush, gonorrhea, fever, arthritis, wounds and infections. Popularly known as merthiolate, it is a plant that belongs to the Euphorbiaceae family. Lectins are proteins capable of binding to carbohydrates and exerting various biological activities such as antimicrobial, insecticide, antitumor and immunomodulatory. The present study aimed to identify, isolate and characterize a lectin extracted from the leaves of J. multifida. Proteins were extracted from leaf by homogenization (16 h, 4 ° C) in three different solutions: 0.15 M NaCl, 50 mM Tris HCl pH 8.0 and 50 mM sodium phosphate buffer pH 7.2. Extraction with 50 mM Tris HCl pH 8.0 showed the highest hemagglutinating activity (AH: 512) as well as the highest protein content (3.15 mg / mL) and higher specific hemagglutinating activity (AHE: 162.44). Confirmation of the presence of lectin was made by the carbohydrate and glycoprotein inhibition of HA, which showed higher specificity to glucose. The obtained extract was treated with ammonium sulfate in different concentrations (0-20%, 20-40%, 40-60% and 60-80%) for protein fractionation and the 0-20% fraction was the only one that presented HA (2048). The 0-20% fraction was subjected to chitin column chromatography equilibrated with 0.15 M NaCl. 2 mL fractions were collected and evaluated for absorbance at 280 nm and HA. A single active protein peak obtained with the 0.5 M acetic acid eluent was pooled and dialyzed against Milli-Q water and 50 mM Tris HCl pH 8.0 for 6 h. To verify the purity of lectin, the sample was analyzed by electrophoretic method in 10% polyacrylamide gel under denaturing conditions, using sodium dodecyl sulfate, and in the presence and absence of reducing agent, where it was possible to visualize a single protein band in the absence of reducing agent. In conclusion, J. multifida leaves are source of glucose-binding lectin.

IDENTIFICATION OF NEW INHIBITORS OF NUCLEOSÍDE HYDROLASE ENZYME FROM LEISHMANIA DONOVANI USING A NEW SCREENING ASSAY

https://proceedings.science/p/120257

Millena Santana Ceroullo [1]; Rodrigo C. da Silva [1]; Isabela T. Ximenes [1]; Lais F. de Carvalho [2]; Maria Cecília B. V. de Souza [1]; Fernanda C. S. Boechat [1]; Luzineide Tinoco [2]; Marcela de Moraes [1]
[1] Universidade Federal Fluminense; [2] Universidade Federal do Rio de Janeiro

A screening assay based on liquid chromatography for LdNH inhibitors was developed. Its application allowed the identification of 12 novel oxoquinoline ribonucleosides as ligands.

Inhibition and binding interactions between acetylcholinesterase enzyme and tyrosine kinase inhibitors

https://proceedings.science/p/122215

Thaís Meira Menezes [1]; Caio Rodrigo Dias de Assis [1]; Roberto Carlos Silva dos Santos [2]; Wilka Karla Martins do Vale [2]; Regildo Max Gomes Martins [3]; Ranilson de Souza Bezerra [1]; Jorge Luiz Neves [1]
[1] Universidade Federal de Pernambuco - UFPE; [2] Universidade Federal Rural de Pernambuco; [3] Universidade Federal do Amazonas

The role of tyrosine kinase inhibitors (TKI) as inhibitors of acetylcholinesterase was evaluated. Enzymatic inhibition and mechanism of interaction were determined by spectroscopic techniques.

Interaction studies in vitro and molecular docking of recreational drugs with ctDNA

https://proceedings.science/p/119915

Camila da Silva Nunes [1]; Wellington Alves de Barros [2]; Karine R. Borges [1]; Carla de A. Vital [1]; Marina de Magalhães Silva [1]; Ângelo Fátima [2]; Josué Carinhanha Caldas Santos [3]; Isis Figueiredo [1]

[1] Universidade Federal de Alagoas; [2] Universidade Federal de Minas Gerais; [3] Universidade Federal de Alagoas

Fluorescence and molecular docking studies revealed that the recreational drugs 25H-NBOMe and 25H-NBOH bind to ctDNA through the interaction of major grooves.

MICROBIOLOGICAL ANALYSIS OF DRINKING-WATER IN PUBLIC SCHOOL IN THE MUNICIPALITY OF SÃO MIGUEL DOS CAMPOS, ALAGOAS STATE, BRAZIL.

https://proceedings.science/p/119812

Micaele Alves da Silva [1]; Vivianne Lins Ebrahim Morcerf [1]; Flávia Bartira Pedro da Silva Almeida [1]; Lázaro Florentino dos Santos [2]

[1] Instituto Federal de Alagoas - IFAL; [2] Universidade Federal de Alagoas - UFAL

Water is only considered potable when is within the limits established by health surveillance; if it is outside these limits, it is considered polluted, it becomes a possible and important means of spreading diseases transmitted via the fecal-oral route. The objective of this research was to present the results of an experimental investigation regarding the microbiological quality of the water consumed in public educational institutions in the municipality of São Miguel dos Campos, Alagoas, Brazil; through the research of Total and Termotolerant Coliforms (fecal) by most probable number (NMP) technique and identification of Escherichia coli and other types of bacteria and fungi in the samples, with the methodology of cultivation in petri dishes, using the means blood agar for the cultivation of bacteria and Sabouraud dextrose agar for the cultivation of fungi. The results of total and thermotolerant coliforms showed that from 12 different schools (100%), it was found that two (16.6%) were in disagreement with the Brazilian potabilityl legislation Nº. 518, March 25, 2004 from the Ministry of Health, in addition, among the 12 (100%) water samples analyzed, 10 (83.3%) presented other types of bacteria or filamentous fungi.

Nitroso-BODIPY as a selective fluorescent probe to glutathione determination

https://proceedings.science/p/120371

Ricardo Alexandre dos Santos [1]; Felipe Silva [1]; Andresa Katherinne Albuquerque de Almeida [1]; Tamires Alves do Nascimento [1]; Marília Oliveira Fonseca Goulart [1]; Josué Santos [1]; Flavio da Silva Emery [2]; Shaiani Gil [2]; Jadriane de Almeida Xavier [1]

[1] Instituto de Química e Biotecnologia (IQB), Universidade Federal de Alagoas (UFAL); [2] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP)

In this work, we describe an application of nitroso-BODIPY dye as a fluorescent probe for a selective determination of reduced glutathione in physiological conditions.

Production of endoglucanase by Penicillium roqueforti ATCC 10110 in a mixture of residues with restrictions

https://proceedings.science/p/120196

Sabryna Couto Araujo [1]; Marla Rosa Marques Ferreira Ramos [1]; Laurieth Góes de Jesus [1]; Luiz Henrique Sales de Menezes [2]; Julieta Rangel de Oliveira [1]; Marcelo Franco [1]

[1] Universidade Estadual de Santa Cruz; [2] Departamento de Ciências Exatas e Tecnológicas, Universidade Estadual de Santa Cruz - UESC, Ilhéus, Brasil

Residues of dendê in SSF. The planning mixtures of waste with restrictions is very effective. The endoglucanase obtained showed an activity of 3,25 U.g-1.

Studies of the antioxidant, antineoplastic profile and interaction with ctDNA of some aminoguanidines derivatives

https://proceedings.science/p/119518

Ari Souza Guimarães [1]; Woodland de Souza Oliveira [1]; Carlos Silva Júnior [1]; Thiago Mendonça de Aquino [2]; Joao Xavier de Araújo Júnior [1]; Pedro Aquino [3]; Aline Rangel Silva Araújo [4]; Ana Lucia Tasca Gois Ruiz; Mary Ann Foglio [5]; Isis Figueiredo [1]; Josué Carinhanha Caldas Santos [6]

[1] Universidade Federal de Alagoas; [2] Chemistry and Biotechnology Institute, Federal University of Alagoas, Maceió, AL, Brazil; [3] Universidade Federal do Agreste de Pernambuco; [4] Universidade Estadual de Campinas; [5] UNICAMP; [6] Universidade Federal de Alagoas

Aminoguanidine derivates showed antioxidant activity against ABTS, DPPH, NO species and FRAP method.PA83 showed promising antiproliferative activity and interacted with DNA preferably via groove mode

Studies related to the shape effect of gold nanoparticles on isolated mitochondria

https://proceedings.science/p/119569

Abner Magalhães Nunes [1]; Reginaldo C. da Silva-Filho [1]; Kleyton R.M. da Silva [1]; Ana Catarina Rezende Leite [1]; Mario Roberto Meneghetti [2]

[1] UFAL; [2] Universidade Federal de Alagoas, Grupo de catálise e Reatividade Química e Instituto de Química e Biotecnologia.

AuNPs have been extensively studied in various biomedical applications due to their unique physicochemical properties. Their properties are strongly dependent on their size and shape. Our previous work showed that rod-like AuNPs were able to affect the mitochondria function. In this present work, we investigated the shape effect of AuNPs on isolated rat liver mitochondria. Spherical and rod-like AuNPs were synthesized and incubated in a 10% BSA solution. The immediate effect of these particles on isolated mitochondria from Wistar rat liver (n = 4) was evaluated. Both morphologies reduced the mitochondrial O2 consumption, specifically in phosphorylative state (nmol/mg/mL): control 43.67 (± 9.68); spheres 26,69 (± 3.70); rods 26.30 (± 4.88); and maximal state (nmol/mg/mL): control 31.28 (± 5.69); spheres 7.20 (± 1.57); rods 8.93 (± 1.61), see Fig. C and D. They also decreased H2O2 production (Fig. E) and the mitochondrial swelling (Fig. F) in c.a. 30%. Under the conditions applied, spherical and rod-like AuNPs showed similar effects in the bioenergetic parameters evaluated, however, rod-like AuNPs were able to dissipate the mitochondrial electrochemical potential and spherical AuNPs were able to keep it, longer than the control (Fig. G). This particular behavior can be related to the shape or to the total surface area of the AuNPs present in the system. To solve this issue, we increased the number of spheres in the medium, reaching then the same surface area found on the rod-like particles system (Fig. I). Now, both systems showed similar effects in mitochondrial potential disruption. All these results shows that AuNPs act on mitochondria bioenergetic process, and particularly, the total surface area of AuNPs in the system is responsible to dissipate or keep the mitochondrial electrochemical potential.

Study of the Aerobic Oxidation Mechanism of Formylhydrazines found in Poisonous Fungi

https://proceedings.science/p/119966

Fabricio dos Santos Senario [1]

[1] Universidade de São Paulo

Study of the Aerobic Oxidation Mechanism of Formylhydrazines found in Poisonous Fungi Some species of edible mushrooms such as the fungus Gyromitra esculenta contain hydrazines, which causes mutagenicity and carcinogenicity in rats [1]. This project aims to study if the oxidation of formylhydrazine (FH) catalyzed by horseradish peroxidase (HRP) generates formyl radical, whose Russel reaction produces singlet oxygen in the aerated medium. Formylhydrazine oxidation catalysis assays were analyzed by spectrophotometry in order to study the effect of the substrate concentration on the system. The oxygen dependence was measured by the oxygrapher, providing data for the construction of a Michaelis-Menten curve, in addition, tests were performed with the addition of superoxide dismutase and catalase to the reaction medium to verify the possible formation of specific intermediates [2]. The HRP cycle, showed the occurrence of the reaction between formylhydrazine and HRP at physiological pH. By oximetry, it was possible to observe the oxygen dependence for the reaction, besides, an enzymatic kinetics curve was constructed, this one showed that the system does not undergo major changes by addition of hydrogen peroxide (H2O2), since there is the formation of the superoxide radical anion (O2•-), which dismutes to H2O2 and activates the HRP, this result was proven by adding superoxide dismutase to the reaction medium, thus decreasing the oxygen consumption speed. [1] Michelot D, Toth B (1991) Poisoning by Gyromitra esculenta – a review. J. Appl. Toxicol. 11: 235-243. [2] Kono Y (1978) Generation of Superoxide Radical during Autoxidation of Hydroxylamine and an Assay for Superoxide Dismutase. Archives of Biochemistry and Biophysics,, 186(1), 189–195.

Synergistic anticancer effect of singlet oxygen and nitric oxide in photodynamic therapy. Application using ruthenium-phthalocyanine compounds

https://proceedings.science/p/119793

Francisco Neto

Synthesis of phenol from acetophenone using whole cells of Geotrichum candidum CCT-1205

https://proceedings.science/p/119782

Taiza Nayara da Silva Caridade [1]; Kelly Teotonio de Sousa [1]; Juliana Alves Vale [1]
[1] UFPB

Fungi are commonly used in biotransformation reactions, because, in addition to containing enzymes that act ascatalysts, their fermentation process is facilitated, promoting the synthesis of compounds with added value in less time than theconventional. In this work, the fungus Geotrichum candidum was used to evaluate the oxidation capacity of the acetophenone substrate and hydrolysis of the phenylacetate ester to form phenol.

Test mixture in LC-HRMS untargeted metabolomics: development and application for urine samples

https://proceedings.science/p/120422

Clarisse Torres [1]; Vinícius Figueiredo Sardela [1]; Fernanda B. Scalco [1]; Francisco Radler Aquino Neto [1]; Rafael Garrett da Costa [1]
[1] Instituto de Química, Universidade Federal do Rio de Janeiro

Visual inspection of pooled QC samples clustering in PCA space do not guarantee reliable LC-MS data. Test mixtures must be used together with pooled QCs in untargeted LC-MS metabolomics.

Unraveling the metabolomics profile of tissues with precursor lesions of cervical cancer

https://proceedings.science/p/120048

Luana Quadros de Souza Leao [1]; Sofia Angiole Cavalcante [2]; Renato Ferreira Hosanah [1]; Marina Amaral Alves [3]; Felipe Mansoldo [4]; Alane Beatriz Vermelho [4]; Rafael Garrett [3]; Priscila F. Aquino [2]
[1] Universidade Federal do Amazonas; [2] Instituto Leônidas e Maria Deane / Fundação Oswaldo Cruz; [3] LADETEC-LABMETA/ Instituto de Química / Universidade Federal do Rio de Janeiro; [4] Departamento de Microbiologia/BIOINOVAR-UFRJ

Untargeted metabolomics approach was able to explore the possible evolution of CINs in Amazonas, showing the differentiation between lesions and adjacent margins and highlighting the histamine.

Whole cells of Geotrichum candidum CCT-1205 applied to the Baeyer-Villiger reaction for the synthesis of ε-caprolactone: Dependence with pH and concentration

https://proceedings.science/p/120041

Kelly Teotonio de Sousa [1]; Renata Rodrigues Magalhães [2]; Taiza Nayara da Silva Caridade [1]; Juliana Alves Vale [2]
[1] UFPB; [2] Universidade Federal da Paraíba

Baeyer-Villiger (BV) oxidation is one of the most important synthesis strategies in fine chemistry, especially in the production of building blocks of optically active lactones with relevant biological applications. In this work the effect of variation of pH and concentration in the conversion of cyclohexanone in caprolactone, were studied concentration of 1, 2 and 3mmol and of pH of 5, 6,5 and 8.

Química de Materiais - MAT

AVALIAÇÃO DA CONDUTIVIDADE TÉRMICA DO COMPÓSITO DE POLIURETANO, CIMENTO COM RESÍDUO DE POLICLORETO DE VINILA

https://proceedings.science/p/120433

Diego Valdevino Marques [1]; Ana Carolina Aguiar [2]; Rachel Faverzani Magnago [1]; Igor Fagundes Valezan [2]; Américo Cruz Júnior Cruz [3]; Luciano Silva [4]

[1] Universidade do Sul de Santa Catarina (UNISUL); [2] UNISUL - Universidade do Sul de Santa Catarina; [3] Universidade Federal de Santa Catarina; [4] Centro de Investigación en Quimica Aplicada

Use of PVC waste for new materials. PU composites with replacement of 50% of primary inputs by residue. Thermal box construction for simple thermal conductivity test.

(Bi13Co12)CoO40/Co3O4 composites: synthesis, structural, vibrational and magnetic characterization.

https://proceedings.science/p/120311

Jefferson Andrey Lopes Matias [1]

[1] Instituto Federal de Educação, Ciência e Tecnologia do Rio Grande do Norte (IFRN)

A theoretical and experimental study of graphene-based three-dimensional nanomaterials for efficient dye removal from water

https://proceedings.science/p/119454

Mayara Bitencourt Leão [1]; José Rafael Bordin [2]; Carolina Ferreira de Matos Jauris [1]

[1] Universidade Federal do Pampa; [2] UFPel

Thermochemical synthesis of 3D materials based on graphene by a simple, low cost and environmentally friendly rot. Theoretical-practical study of the adsorption of methylene blue in water.

A theoretical-experimental study of factors influencing the characteristics and properties of macroporous graphene-based materials decorated with silver particles

https://proceedings.science/p/119646

Paulo Castro Cardoso da Rosa [1]; Mayara Bitencourt Leão [1]; Anna Elisa Silva [2]; Eduardo Guilherme Cividini Neiva [2]; José Rafael Bordin [3]; Carolina Ferreira de Matos Jauris [1]

[1] Universidade Federal do Pampa; [2] Fundação Universidade Regional de Blumenau (FURB); [3] Universidade Federal de Pelotas

Simple changes in the synthesis route of porous macrostructures based on graphene and silver particles provide the formation of materials with extremely different characteristics and properties.

Adsorbent magnetic materials based on green coconut husks biochar and superparamagnetic iron oxides

https://proceedings.science/p/120340

Bruno Salarini Peixoto [1]; Beatrice Muzzi [2]; Martin Albino [3]; Michele Petrecca [3]; Gilberto Alves Romeiro [4]; Marcela de Moraes [4]; Claudio Sangregorio [5]

[1] Universidade Federal Fluminense; [2] Università degli Studi di Siena / Dipartimento di Biotecnologie, Chimica e Farmacia; [3] Università degli Studi di Firenze / Dipartimento di Chimica "Ugo Schiff"; [4] Universidade Federal Fluminense / Instituto de Química / Departamento de Química Orgânica; [5] Consiglio Nazionale delle Ricerche / Istituto di Chimica dei Composti Organometallici

High specific surface area mesoporous biochar was synthesized by slow pyrolysis using H3PO4. The composite prepared using SPION supported on the biochar is easily separated from water using a magnet.

Analysis of thermochromatic inks and thermochromatic thin films with precise temperature control to be used as temperature sensors

https://proceedings.science/p/119991

Daniel Aparecido Pires [1]
[1] Universidade de Franca (Unifran)

Avaliação do uso da Própolis Vermelha de Alagoas (PVA) como inibidor de corrosão

https://proceedings.science/p/120339

Williams Raphael de Souza Morais [1]; Jaceguai Soares da Silva [2]; Carmem Lucia Zanta [3]; Ticiano Gomes do Nascimento [3]; Josealdo Tonholo [3]
[1] CETEC/UFAL; [2] Instituto Federal de Educação, Ciência e Tecnologia do Amapá; [3] Universidade Federal de Alagoas

The ethanol extract of Red Propolis of Alagoas was evaluated as a corrosion inhibitor in carbon steel and presented itself as a good inhibitor reducing the corrosion parameters.

Beads of Al-MCM-41 dispersed in sodium alginate matrix for dye adsorption from aqueous solution

https://proceedings.science/p/120072

Maria Vitória Lima Ramos [1]; Adonay Loiola [2]; Natalia Porto Alexandre [2]; Édipo Silva Oliveira [2]
[1] Universidade Federal do Ceará; [2] UNIVERSIDADE FEDERAL DO CEARÁ

Al-MCM-41 matrix hierarchized with sodium alginate for the adsorption of dyes;
Kinetic study of methylene blue dye to verify the adsorptive capacity of the hierarchical material

Bioavailability of macronutrient incorporated in nanostructures for application in agriculture

https://proceedings.science/p/120418

Yolice Moreno Ruiz [1]; Camila Pereira [2]; Helena Bonilla [2]; James Correia de Melo [1]; Andre Galembeck [3]
[1] Centro de Tecnologias Estratégicas do Nordeste; [2] Universidade Federal de Pernambuco - UFPE; [3] UNIVERSIDADE DE PERNAMBUCO

In this work, the macronutrients (potassium, phosphorus, and nitrogen) have been incorporated into chitosan and silica nanoparticles and delivered to sugarcane raised by tissue culture.

Biodegradable matrices based on Poly (3-hydroxybutyrate) (PHB) and Starch for programmable release fertilizer coating

https://proceedings.science/p/119776

Débora França [1]; Roselena Faez [2]
[1] Universidade de São Paulo - FZEA; [2] Universidade Federal de São Carlos
Natural and biodegradable polymers are applied to smart material for agriculture. Reducing the coatings residue of fertilizers on the soil.

BIPHASIC ZIRCONIA APPLIED IN ENVIRONMENTAL REMEDIATION BY DECOLORATION OF SOLUTIONS CONTAINING INDUSTRIAL DYES

https://proceedings.science/p/120614

João de Jesus Maurício [1]; Ieda Maria Garcia dos Santos [2]
[1] Departamento de Química / Centro de Ciências Exatas e da Natureza / Universidade Federal da Paraíba; [2] Núcleo de Pesquisa e Extensão/ Laboratório de Combustíveis e Materiais, UFPB

The zirconium oxide was synthesized by the modified Pechini method and proved to be effective in decoloration of industrial dye solutions.

CAPTURA DE CO2 EM ADSORVENTES DERIVADOS DA CARBONIZAÇÃO HIDROTÉRMICA DA QUITOSANA

https://proceedings.science/p/120296

José Adolfo Oliveira das Chagas [1]; Bianca P. Pinto [1]; Claudio J.A. Mota [1]
[1] IQ-UFRJ

A quitosana, um heteropolissacarídeo obtido a partir da N-desacetilação da quitina, tem se destacado como matéria-prima para produção de carvões adsorventes de CO2 [1], [2]. Isso se deve a interação ácido-base entre a molécula de CO2 e os grupos amino na estrutura dos materiais derivados da quitosana (Fig. 1). Neste trabalho, relatamos a carbonização hidrotérmica da quitosana e os efeitos do tempo de reação (1-48h) nas propriedades químicas dos materiais, bem como a potencialidade destes na captura de CO2. A carbonização hidrotérmica da quitosana foi realizada a 180°C e os materiais obtidos foram caracterizados por diferentes técnicas, tais como, análise elementar CHN, espectroscopia no Infravermelho (IV), Ressonância Magnética Nuclear de 13C (RMN), titulação de Boehm, análise textural e Microscopia Eletrônica de Varredura (MEV). A análise elementar CHN indicou que, em comparação com a quitosana, os materiais HTC apresentaram um aumento do teor de carbono e redução da quantidade de oxigênio, devido a desidratação do polímero durante o tratamento. No entanto, o teor de nitrogênio não variou significativamente com o tempo de reação, indicando que a carbonização hidrotérmica não leva à perda significativa do conteúdo de nitrogênio. Pelas análises de IV verificou-se a diminuição da banda de estiramento OH e o aparecimento de bandas associadas a ligações aromáticas em C-N e C-O para os materiais tratados. Adicionalmente, a análise de RMN de 13C confirmou a natureza mais aromática dos adsorventes com o tempo do HTC. Pela titulação de Boehm foi observado que ocorre uma redução da basicidade dos hidrocarvões com o tempo de tratamento. Essa redução é mais acentuada para os materiais tratados em tempos mais longos e pode estar associada à formação de aminas aromáticas, que são bem conhecidas por serem bases mais fracas. Embora não tenham apresentado mudanças significativas na área superficial, os hidrocarvões exibem uma morfologia irregular com pequena distribuição de poros, de acordo com análise de MEV. Dessa forma, o efeito sinérgico, entre as mudanças na composição, estrutura química e morfologia da quitosana com o tempo da carbonização hidrotérmica, promoveu o aumento da capacidade de adsorção de CO2 na ordem de 4 vezes.

Carboxymethylation of Delonix regia Galactomannan

https://proceedings.science/p/120260

Francisco Joan Gonçalves Pontes [1]
[1] UFCE

Cashew gum as a sol-gel precursor for green synthesis of nanostructured Ni and Co ferrites (MFe2O4, M = {Ni, Co}).

https://proceedings.science/p/120177

Evanimek Bernardo Sabino da Silva [1]
[1] Universidade Federal do Rio Grande do Norte

Cashew gum sol-gel precursor.
Green synthesis nickel and cobalt ferrite nanoparticles.

Cation-exchanged Zeolite A/alginate beads for biogas upgrading

https://proceedings.science/p/120488

Jadson Bernardino Guedes [1]; Adonay Loiola [2]; João Batista Araújo da Silva Júnior [3]; Raquel de Andrade Bessa [1]; José Demontier Vieira de Souza Filho [4]; Franscisco Suetonio Batos Mota [4]

[1] Departamento de Química Orgânica e Inorgânica / CENTRO DE CIÊNCIAS / UNIVERSIDADE FEDERAL DO CEARÁ; [2] UNIVERSIDADE FEDERAL DO CEARÁ; [3] Centro de Ciências e Tecnologia da Região dos Inhamuns / CECITEC / UECE; [4] Departamento de Engenharia Hidráulica e Ambiental / CENTRO DE TECNOLOGIA / UNIVERSIDADE FEDERAL DO CEARÁ

Zeolite (Na+, Ca2+, K+ and Ag+)A, was synthesized via hydrothermal route; Zeolite/alginate beads were prepared, in order to analyze the performance of the CO2 adsorption in landfill biogas.

Cellulose acetate mats from DMAc/THF solutions: Optimization of electrospinning parameters

https://proceedings.science/p/120593

Thamiris Voltarelli Ferracini [1]; Rachel Passos de Oliveira Santos [1]; Elisabete Frollini [1]

[1] Macromolecular Materials and Lignocellulosic Fibers Group/ Center of Research on Science and Technology of BioResources/ Institute of Chemistry of Sao Carlos/ University of Sao Paulo

Objective: to optimize electrospinning of DMAc/THF cellulose acetate(CA) solutions.
11 wt%CA, DMAc/THF:35/75, 20kV, 20 cm, 5 µL.mL-1->network of ultrathin bead-free fibers and good tensile properties.

Characterization and use of nanocomposite obtained from atapulgite and zero-valent iron for the degradation of metronidazole in water

https://proceedings.science/p/120166

Rafael Mendes Coelho [1]; Débora Vilela Franco [1]; Edivaldo dos Santos Filho [1]; Leonardo Morais da Silva [1]; Maria Eduarda Soares Pinheiro [1]

[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Application and characterization of zero-valent iron supported on attapulgite for the removal of metronidazole in water using oxone. Zero-valent iron for PMS activation. Degradation of contaminants.

Characterization of colloidal metallic nanoparticles by microwave-assisted decomposition platform

https://proceedings.science/p/120212

Naiara Vieira Godoy [1]; Rodrigo Moretto Galazzi [1]; Katherine Chacón-Madrid [1]; Marco Arruda [1]; Italo Odone Mazali [1]

[1] Universidade Estadual de Campinas

Development of a microwave-assisted decomposition platform to real Au content determination in single- and multi-elemental metallic nanoparticles in complex matrices by ICP-MS and OES

Chelate intercalating-LDH for trace metal removal

https://proceedings.science/p/120117

Luiz Fernando Brum Malta; Caio Gentil Nascimento Silva [1]

[1] UFRJ

LDH materials are based on a metallic M2+/M3+hydroxide layered network. The interlayer space is occupied by anions to balance the intralayer positive charge therefore being anion exchangers. Such property allows inserting anionic species giving rise for instance to heavy metal removers1. To best accomplish this task the layered structure must display high surface area, crystallinity and low carbonate content (for the ease of ion exchange).Starting from a LDH Mg:Al whose synthesis was already optimized by a previous study, this material was submittedto

hydrothermaltreatment at 80oCunderN2 atmosphere. Theanionic species inserted were tartrateion and EDTA (ethylenediamine tetraacetic acid)at pH=7. It was used a 22factorial design for the process optimization. The varied parameters were those of Table 1. Samples were characterizedby X-Rays Diffraction (XRD),Fourier-transform infrared spectroscopy (FTIR)andThermogravimetric analysis (TGA). The outcomes to be evaluatedwere the presence of EDTA or tartrate bands in FTIR spectra; dislocation of 003 peak in XRD patterns; and mass loss % relative to intercalated organic anions by TGA.Intercalation experimentsrevealed that EDTA leadedthe LDH's layerstowards collapsesince low yields of the final material were achieved (~10%).However the tartrate insertion was effected in all experiments accordingtoFTIR resultsthat evidenced COO stretching mode at 1585 cm-1.TGA curves pointed to the highest mass loss of 54% relative to the set of intercalation conditions of 6h and 253 K. Therefore these were considered the best conditions for tartrate intercalation.XRD patterns of these samples are still in progress.

Controlled Release Study of Pharmaceuticals Adsorbed in Cellulose/Ionic Liquid Grafted Matrix

https://proceedings.science/p/119708

Marcelo Gomes Speziali [1]; Beatriz Sencovici de Oliveira [1]; Stefânia Sales de Oliveira Santos [1]
[1] Universidade Federal de Ouro Preto

Conversão de luz em eletricidade utilizando células a combustível fotocatalíticas de ditionito-perclorato

https://proceedings.science/p/120498

Antero Ricardo Santos Neto [1]; Camila Almeida Fernandes Souza [1]; Izabela Campos Sena [2]; Marcio Cesar Pereira [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri; [2] UFVJM

A W-BiVO4-Pt photoelectrochemical cell that uses perchlorate as an electron acceptor consumes dithionite fuel to convert light into electricity with a power density of 4.2 mW cm-2.

Curcuminoids encapsulated in nanoemulsions stabilized by kefiran: preparation and characterization

https://proceedings.science/p/120442

Matheus da Silva Campelo [1]; Denise Ramos Moreira [1]; Nágila Maria Pontes Silva Ricardo [1]; Maria Elenir Nobre Pinho Ribeiro [1]
[1] Universidade Federal do Ceará/Centro de Ciências/Departamento de Química Orgânica e Inorgânica

Curcuminoids (isolated from turmeric rhizomes) were encapsulated in a nanosystem stabilized by kefiran (isolated from kefir grains);
The nanoemulsions showed excellent colloidal stability for 30 days.

Deposition of mixed metallic nanoparticles coated with a luminescent complex on the silica substrate, a potential application for optical sensors.

https://proceedings.science/p/119976

Renata Adati [1]; Marcela Oliveira [1]; Amanda Pereira [1]
[1] Universidade Tecnológica Federal do Paraná

Deposition of mixed metallic nanoparticles coated with a luminescent complex on the silica substrate that allows the production of optical sensors.

DESIGN DE UM NOVO MATERIAL CONVERSOR DE LUZ A BASE DE Eu3+ COMBINADO COM O LIGANTE NATURAL LAPACHOL E (EuDBM)3.2H2O

https://proceedings.science/p/120141

Andrei Marcelino Sá Pires Silva [1]; Jorge Fernando Silva de Menezes [1]; Suellen Maria Valeriano Novais [1]; Gabriel Prazeres Useda [1]; José Gabriel Santos Barbosa [1]

[1] UFRB

In presente work, we carried out the synthesis of a Eu3+ -dibenzoylmethanate complex that integrates the natural ligand Lapachol, as an inexpensive alternative that potentially amplifies the emission.

Development and characterization of materials involving Photoactive Tungstic Keggin Species on Faujasite Y Zeolite

https://proceedings.science/p/120426

Mateus Freitas Paiva [1]; Silvia Cláudia Loureiro Dias [1]; José Alves Dias [1]

[1] Universidade de Brasília

An extensive structural and physicochemical characterization showed the generation of new catalytic materials with better activity properties (lower band gap values and higher acidity).

Development of photoelectrochemical device based on W-BiVO4 and V2O5 for solar energy conversion into electricity or chemical energy.

https://proceedings.science/p/120243

Izabela Campos Sena [1]; MARCIO CESAR PEREIRA [1]

[1] UFVJM

Development of photoelectrochemical device based on W-BiVO4 and V2O5 for solar energy conversion into electricity or chemical energy. The work is based on the synthesis and characterization of semiconductors based on W-BiVO4 and V2O5 until their characterization, later forms of deposition and the viability of an extra layer of W-BiVO4 are tested to delay the corrosion effect and increase the efficiency of the complete cell. In addition, the electrolyte solutions used have not yet been reported in further work.

Dispersão Sólida de Efavirenz em Amido Poroso

https://proceedings.science/p/120634

Jackson Antonio L. C. Resende [1]; Karynne C. de Souza [1]; Arturo B. L. Véliz [1]

[1] Universidade Federal de Mato Grosso

- FTIR and SEM describe the presence of Efavirenz in the starch matrix; - DSC and DRX have no crystalline EFV peaks; - Porous starch soluble as amorphizing agent of Efavirenz

Downshift red-near-UV-excited LEDs based on Ir-complexes with Schiff bases

https://proceedings.science/p/119612

Sergio A Marques de Lima [1]; Felipe da Silva Manrique Canisares [2]; Airton Germano Bispo-Jr [1]; Ana Maria Pires [3]

[1] Universidade Estadual Paulista-Unesp; [2] Instituto de Química - UNESP; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Keywords: Schiff bases, iridium complexes, luminescence, solid-state lighting, WLEDs. Highlights The near-UV-to-red downshifting converter Ag[Ir(ppz)2(BS1)] complex may be used as coating of near-UV-excited warm WLEDs due to the high emission color purity and the high photostability. Abstract Ir-based complexes find several applications such as in catalysis, optoelectronics, biomedicine, solar energy conversion as well as in solid-state lighting (SSL).[i] Focusing our attention on SSL, Ir-based complexes can be used as coatings of near-UV-excited light-emitting diodes (LEDs) towards the fabrication of warm white-emitting LEDs (WLEDs) due to their strong absorption within the near-UV region and tunable light emission.[ii] Although a couple of blue or green-emitting Ir complexes featuring high emission quantum yield have already been reported[iii], there is a lack of near-UV-to-red downshifting converter Ir-

complexes[iv]. In this context, herein, we introduce the synthesis of two Schiff base ligands and their red-emitting Ir-complexes in order to evaluate their use as coatings of near-UV-excited LEDs. The Schiff bases 2-(((3-methyl-1-phenyl-1H-pyrazol-5-yl)imino)methyl)phenol (BS1) and 5-(diethylamino)-2-(((3-methyl-1-phenyl-1H-pyrazol-5-yl)imino)methyl)phenol (BS2) were synthesized via condensation reaction of a primary amine and an aldehyde. Those ligands were used to synthesize the Ag[Ir(ppz)2(BS1)] and Ag[Ir(ppz)2(BS2)] complexes (ppz = phenylpyrazole) through the reaction with the Ir-precursor, [(ppz)2Ir(μ-Cl)Ir(ppz)2], in dichloromethane at 46°C, assisted by Ag2O. The structures of BS1, BS2, and their respective Ir-complexes were elucidated by FTIR, UV-Vis, elemental and thermal analysis, 1H-NMR, and/or MALDI-TOF. Under UV excitation, the ligands exhibit emission in the yellow (BS1) and in the green (BS2). On the other hand, under UV excitation, both Ag[Ir(ppz)2(BS1)] and Ag[Ir(ppz)2(BS2)] emit a broadband centered at 627 and 604 nm, and 1931CIE color coordinates of (0.659;0.337) and (0.612;0.380), respectively, both within the red spectral region, with 100 % of color purity. Since Ag[Ir(ppz)2(BS1)] exhibits red color coordinates ideal for warm WLEDs, it was used to coat a commercial near-UV-emitting LEDs (395 nm), the ligand BS1 was also investigated for comparison. The two LED prototypes emit in the yellow (BS1) and in the red (Ag[Ir(ppz)2(BS1)]) spectral regions. Moreover, inasmuch as the application of the complexes in SSL depends on their reliability, the radiant photostability of the as-fabricated LEDs were overseen for 24 h of operation at 2.9 V. The BS1-LED prototype featured an intensity decrease of 60 % after 24 h while the intensity of the Ag[Ir(ppz)2(BS1)]-LED decreased only 10 %, confirming that the complex features near-UV-to-red conversion and photostability desired for application as warm WLED. Acknowledgments Capes (88887.341772/2019-00), CNPq(304003/2018-1) and Fapesp (2015/03400-5). [i] Meng, G.; Chen, Z.; Tang, H.; et. Al., Z. 2015, 39, 9535–9542. [ii] Chen, M.; Sun, R.; Ye, Y.; et. Al., Opt. Mater. 76 (2018)141–146. [iii] Hyun, J., Young, S., Kim, K., Thin Solid Films 517 (2009) 1807–1810 [iv] Chen, M.; Sun, R.; Ye, Y.; et. Al., Opt. Mater. 76 (2018)141–146.

Drug delivery system based on reduced graphene oxide functionalized with host-guest complex between cationic pillar[5]arene and an anti-leishmania drug

https://proceedings.science/p/119624

Isabela Alves de Albuquerque Bessa [1]; Tamires Soares Fernandes [1]; Thiago Custódio dos Santos [1]; Vanessa do Nascimento [2]; Célia Machado Ronconi [3]
[1] Química Inorgânica / Instituto de Química / Universidade Federal Fluminense; [2] Universidade Federal Fluminense - UFF; [3] Universidade Federal Fluminense

A new drug delivery system based on reduced graphene oxide and a cationic pillar[5]arene loaded with miltefosine, a drug to treat leishmaniasis.

EFEITO DA TEMPERATURA DE SÍNTESE NA CRISTALINIDADE DE HDL, MgX-Al-CO3, NiX-Al-CO3 x= 2 e 3, POR DIFRAÇÃO DE RAIOS X.

https://proceedings.science/p/119659

Lucas Vieira de Souza [1]; Luiza Cristina de Moura [1]; Meri Domingos Vieira [1]
[1] Universidade Federal do Rio de Janeiro

The influence of digestion temperature on the synthesis of LDH Mg-Al and Ni-Al intercalated with carbonate ions has been studied in order to observe the effects on crystallinity of the samples.

Electrochemical water oxidation by Prussian blue analogues studied by a 3D printed scanning electrochemical microscope (SECM)

https://proceedings.science/p/119643

Rafael Lavagnolli Germscheidt [1]; Gabriel de O. [2]; Andre Formiga [2]; Tulio C. R. da Rocha [3]; Juliano A. Bonacin [2]
[1] Universidade de Campinas - Unicamp; [2] Universidade de Caminas - Unicamp; [3] Laboratório Nacional de Luz Síncrotron

As the global demand for energy has increased in the past few decades, the search for new sources of green energy has become an important topic. Among the substantiable energy sources, a good way to address this problem is storing energy in the form of chemical bonds, such as H2, which can react with oxygen, producing only water vapor. Hydrogen can be obtained from different sources, thus, one interesting way to obtain this product is from the water splitting reaction, however the bottleneck reaction in water splitting is the water oxidation, therefore, cost-effective catalysts

have been researched in the past years, and among them, Prussian blue analogues (PBA) had stood out due to its great performance and stability in pH 7. Nevertheless, understanding the mechanism in a full way, still remains a challenge. Scanning electrochemical microscopy (SECM) is an electrochemical tool that is wildly used to probe surface reactions, working for both quantitative and qualitative analysis. SECM has been used to study water oxidation reaction (WOR) on the substrate generation-tip collection (SG-TG) mode, where the tip is a probe that reduces the O2 produced by the catalyst, being able to identify spots and catalysts that have a higher production of oxygen. In this work, we developed a 3D printed scanning electrochemical microscope and used it to monitor the WOR for different PBA supported on glassy carbon electrode (GCE), comparing their performances during this reaction. The platinum tip electrode was calibrated with a dissolved oxygen (DO) sensor (Hanna inst.) so the real concentration of evolved O2 could be obtained, and therefore, turnover frequencies (TOFs) could be calculated to have real insights on their performances.

Enhanced removal of methylene blue from aqueous solution using polyacrylamide/aminated graphene oxide hydrogels

https://proceedings.science/p/119608

Marcelo Machado Viana [1]; Sthéfany Z S do Amparo [1]; Meiriane C F S Lima [1]; Raquel C F G. Lopes [1]; Cláudia K B Vasconcelos [2]; Vinicius Caliman [1]; Glaura Goulart Silva [1]

[1] Universidade Federal de Minas Gerais; [2] Pontifícia Universidade Católica de Minas Gerais

Few layers graphene oxide (GO), graphene oxide functionalized with diethylenetriamine (GO-DETA) and the hybrid of graphene oxide-diethylenetriamine and polyacrylamide (GO-DETA/PAM) hydrogel with high adsorption of methylene blue were prepared using microwave-assisted methods. TGA and XPS analysis were performed to confirm DETA molecules incorporation on GO and to identify an in-situ acrylamide polymerization with no usual chemical cross-linkers. The morphology and structure of the graphene derivative materials and hybrid gel were evaluated by TEM and SEM images. The obtained GO-DETA sheets played an important role as a cross-linker agent during the polymerization of PAM to form the hybrid GO-DETA/PAM. The results obtained showed that the GO-DETA influenced the swelling behavior and thermal properties of PAM, as well as improved its Tg, presenting a more stable PAM network in saline conditions. The hybrid hydrogel significantly improved the capacity to adsorb methylene blue (maximum adsorption capacity 205.4 mg / g), compared to the neat PAM (maximum adsorption capacity 51.5 mg / g). This feature demonstrates how this novel material can be used in the removal of emerging contaminants in water, for example, using a fast and reproducible synthetic method and lower quantities of adsorbent.

Enhanced-efficiency phosphorus fertilizer based on seaweed polysaccharides reinforced with cellulose nanofibers

https://proceedings.science/p/119417

Gabriella Ulrich [1]; Roselena Faez [2]

[1] Faculdade de Zootecnia e Engenharia de Alimentos (FZEA/USP); [2] Universidade Federal de São Carlos

Global technological development is linked to the needs of society and, given the exponential increase in population, agrarian expansion has gained prominence due to the use of large-scale fertilizers. The design of materials with effective properties that aid agricultural development has gained prominence in recent decades, mainly inputs for the quantified and prolonged release of nutrients used in different cultures in Brazil. This project studies the formation of composite films between K-carrageenan and alginate, attractive polysaccharides due to environmentally favorable properties and low cost to obtaining, with an increment of nutrient ammonium dihydrogen phosphate (ADP) and reinforced with cellulose nanofibers (CNF) at different concentrations, in order to act as a support and release of nutrients in a programmed way. Init.ially, a study was developed about the best proportion among the Kc / Alg constituents using the casting technique, obtaining the 40/60 polymer fraction as a response. To this composition, CNF (1, 2, and 4%) and ADP (12%) fractions in relation to the dry mass of the materials were added to this composition (Figure 1). Satisfactory results were obtained through swelling and thermal analysis for composition 40Kc/60Alg/4%CNF/ADP (Figure 2), observing films with good thermal stability and best properties for swelling. Thus, the study of new materials with high added value, coming from sustainable, renewable, and abundant sources, is strategic not only from a technological/economic point of view but also environmental, due to the reduction of damages caused by the use excessive amount of fertilizers in Brazilian crops.

Estudo da Funcionalização de Grafenos Quimicamente Esfoliados com Polímero Condutor

https://proceedings.science/p/120612

Laura Paulinelli [1]
[1] Comissão Nacional de Energia Nuclear

Functionalization strategy between graphenes and conductive polymer. Graphenes produced via chemical exfoliation route. Conductive polymer synthesized via chemical route.

ESTUDO DA TRABALHABILIDADE DE COMPÓSITOS HIDROGEL-CIMENTO

https://proceedings.science/p/120520

Giovanni Souza Casella [1]; Thalles Vilela [1]; Matheus Santos [1]
[1] Pontifícia Universidade Católica de Minas Gerais - PUC Minas

Hydrogel are known for their high absorption power and their controlled liberation of fluids. Those capacities can likely be seized to improved cement structural formation.

Estudo preliminar de ensaios físico-mecânicos de compostos de borracha utilizando plastificante de origem vegetal e sistema de cura peroxídica para utilização em correias transportadoras.

https://proceedings.science/p/120479

Valéria Dias [1]; Julia Buci [2]; Nella Nelci Mussugati de Jesus [2]; Thiago Jacinto de Pádua [3]
[1] UNIFACCAMP - Centro Universitário Campo Limpo Paulista; [2] Universidade de São Paulo; [3] Centro Universitário Campo Limpo Paulista

Thermal Stability

Best thermal resistance, best physical properties. Peroxidic reticulation are more stable than the conventional cure with sulfur.

Evaluation of the antioxidant capacity of hybrid nanoparticles containing selenium and copper in different stabilizing agents

https://proceedings.science/p/119519

Woodland de Souza Oliveira [1]; Maria de Fátima C. da S. Neta [2]; Josué Carinhanha Caldas Santos [3]; Cintya D. E. S. Barbosa [2]; Daniela Santos Anunciação [2]
[1] Universidade Federal de Alagoas; [2] UFAL; [3] Universidade Federal de Alagoas

Selenium nanoparticles (SeNPs) have anti-cancer, antioxidant, antibacterial and anti-inflammatory action and these properties can be enhanced through association with other elements.1 The present work aimed to evaluate the antioxidant capacity (CAO) of SeNPs and hybrid Se and Cu nanoparticles (SeCuNPs), previously synthesized and characterized in different polymeric stabilizing agents. The NPs were synthesized based on the adapted literature with chitosan (QUI) and polyvinyl alcohol (PVA) as stabilizing agents.2 Once synthesized and characterized, the ABTS assay was performed to assess the antioxidant capacity of NPs. For this purpose, analytical curves were constructed with NPs and stabilizing agents. The results were expressed as a function of IC50 (concentration required to inhibit 50% of ABTS●+) and compared with Trolox (phenolic compound) and ascorbic acid (reducer) standards. Fig. 1 (a - d) represents the shape and size of the NPs obtained by transmission electron microscopy (TEM), in which there is a reduction in the size of SeCuNPs in relation to SeNPs, regardless of the stabilizing agent. However, this size variation resulting from the differentiated nucleation step in the presence of copper, was more expressive in QUI (from 94 to 36 nm). The CAO results of the synthesized NPs (Fig., 1e) showed high CAO with IC50 between 0.3 and 0.4 mg L-1 , 81-85% more efficient than the Trolox and ascorbic acid standards. The QUI and PVA stabilizers showed inhibitions lower than 10% at concentrations up to 200 mg L-1 . From the data obtained, it can be inferred that the synthesis of hybrid Se and Cu NPs promoted a reduction in size compared to SeNPs, in addition to presenting high antioxidant capacity, thus enabling applications in biological systems. Thus, further tests to assess the antioxidant capacity will be carried out to obtain complementary data on the hybrid material, for example, the ferric reducing antioxidant power (FRAP) and DPPH● radical scavenging capacity.

Facile solvent-free synthesis of mesoporous carbon: an efficient adsorbent for 17α-ethinylestradiol

https://proceedings.science/p/119667

Rayane Cristian Ferreira Silva [1]; Ana Paula de Carvalho Teixeira [2]; Paula Sevenini Pinto [3]
[1] Universidade Federal de Minas Gerais ; [2] Universidade Federal de Minas Gerais; [3] Universidade Estadual de Minas Gerais/Divinópolis

Synthesis of mesoporous carbon. Solvent-Free method. Adsorption of the 17α-Ethinylestradiol

Filmes finos e avanços em sistemas nanoestruturados

https://proceedings.science/p/120695

Renata Adati [1]
[1] Universidade Tecnológica Federal do Paraná

O estudo de propriedades de novos materiais na escala nanométrica tem despertado cada vez mais o interesse dos grupos de pesquisa, assim o desenvolvimento de técnicas que possibilitam a obtenção de materiais orgânicos e/ou híbridos nesta escala é de extrema importância; para filmes nanométricos estruturados por exemplo, destaca-se as técnicas de: Langmuir-Blodgett (LB) e Automontagem: Self-Assembly (automontagem) e Layer-by-Layer (camada por camada). N esta apresentação será abordada a técnica de LB utilizada para o estudo de monocamadas ou filmes de Langmuir, exploradas com sucesso devido as peculiaridades como: i) propriedades interfaciais controladas por ação mecânica, e ii) controle no processo de transferência e deposição de multicamadas, especialmente para o desenvolvimento de nanomateriais de preciso controle molecular como sensores e dispositivos ópticos.

Fluorescent Organic-Inorganic Hybrid Materials based on Benzothiadiazole Bridged Silsesquioxanes

https://proceedings.science/p/120492

Marieli Rodrigues [1]; Victória Goulart Isoppo [1]; Lucas Zielinski do Canto [1]; Angélica Moro [1]; Fabiano Severo Rodembusch [1]
[1] Universidade Federal do Rio Grande do Sul

Photoluminescent bridge silsesquioxane precursors have a wide range of applications, due to their potential in the development of new organic-inorganic hybrid materials. Particularly, its fluorescent.

Fuels production by thermal decomposition of nickel oleates

https://proceedings.science/p/119942

Vivian Andrade Luciano [1]; Marcelo Gonçalves Rosmaninho [2]; Ana Paula de Carvalho Teixeira [1]
[1] Universidade Federal de Minas Gerais; [2] Universidade Federal de Ouro Preto

Thermal decomposition of nickel oleates; Formation of gaseous products of industrial interest, mainly type C4 hydrocarbons.

Gel polymer electrolyte system based on Agar-Agar doped with Ionic Liquid

https://proceedings.science/p/120171

Larissa Agostinho de Santa Cruz Oliveira [1]; Fabiele Collovini Tavares [2]; Rhauane Almeida Galvao [1]; Giovanna Machado [3]
[1] Universidade Federal de Pernambuco - UFPE; [2] Universidade Federal do Rio de Janeiro; [3] Centro de Tecnologias Estratégicas do Nordeste

• Conductive biopolymer based on Agar-Agar; • Agar-Agar doped with ionic liquid; • Electrostatic interaction; • Gel electrolyte for solar cells and batteries.

Gold nanorods assembled in microfabricated channels: three-dimensional SERS hotspot matrix

https://proceedings.science/p/120143

Jaciara Bär [1]; Anerise de Barros [1]; Davi Henrique Starnini de Camargo [2]; Mariane Peres Pereira [2]; Fernando Aparecido Sigoli [1]; Carlos Bufon [2]; Italo Odone Mazali [1]

[1] Universidade Estadual de Campinas; [2] (CNPEM) Centro Nacional de Pesquisa em Energia e Materiais

SERS substrate development for analyte detection at ultra-low concentrations. Assembled of AuNRs using “V” shaped channels to SERS application. Three-dimensional SERS hotspot matrix.

Green synthesis of silver nanostructures using amino acid functionalized Pluronic F127 and evaluation of their antibacterial action

https://proceedings.science/p/120343

Douglas Costa Santos [1]; Diego Fonseca Bispo [1]; Viviane Costa de Souza [1]; George Ricardo Santana Andrade [2]; Euler Araújo dos Santos [1]; Zaine Teixeira Camargo [1]

[1] Universidade Federal de Sergipe; [2] Universidade Federal do Espírito Santo

The increasing number of antibiotic-resistant bacteria has become a challenge for contemporary medicine. Nanotechnology brings new possibilities in effectively combating multi-resistant bacteria, in which one of the most promising system is the silver nanostrutuctures (SNS) that can be associated with polymers for biomedical use. Herein, Pluronic F127 was functionalized with amino acids in obtaining and stabilizing of SNS. The amino acids glycine, L-Alanine and DL-Alanine were used in the esterification reaction of the PEO end groups present in the polymer chain. These polymers were used in the reduction of Ag+ ions and in the stabilization of the nanoparticles by the hydrothermal and the photosensitization routes. The functionalized polymers were characterized by FTIR, in which esterification probably occurred since bands of amine groups was observed, while the stretching band of carbonyl groups from amino acids (-C=O) was absent. SNS were characterized by UV-Vis absorption spectroscopy and by TEM analyze. The SNS obtained by the hydrothermal route are predominantly spherical, whereas those obtained by photosensitization give rise to rods and prisms. Analyses by Fluorescence confirmed that metal clusters were present in the samples obtained by photo-assisted method using glycine and D.L-alanine. The SNS obtained by photo-assisted route were efficient against S. aureus, evaluated by the well diffusion method, in which the ones containing clusters presented larger zones of inhibition.

Heavy-metal oxide glass containing Te0 nanoparticles and CdS quantum-dots for photonic applications

https://proceedings.science/p/120255

Danilo Manzani [1]; Renato G. Capelo [2]; Valmor R. Mastelaro [2]; Giulia A. dos Santos [2]; Vinicius Leonardo Souza [2]

[1] Instituto de Química de São Carlos, Universidade de São Paulo (IQSC-USP), Departamento de Química e Física Molecular; [2] USP - São Carlos

Controlling the synthesis in-situ of Te0 and CdS quantum dots in tellurite and fluorophosphate glass induced by sulfide precursor and fs-laser irradiation for the fabrication of waveguides.

Hierarchical films based on bacterial celullose and Ca2+, Cu2+, Zn2+-exchanged zeolite A for controlled release of NO

https://proceedings.science/p/120060

Natalia Porto Alexandre [1]; Adonay Loiola [1]; Matheus Barros [2]; Armando Diego .I. Freitas [3]; Russell Morris [4]; José Marcos Sasaki [1]; Simon M. Vornholt [4]; Morven J, Duncan [4]; Morsyleide de Freitas Rosa [5]

[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Instituto Federal de Educação, Ciência e Tecnologia do Ceará; [3] Departamento de Química Orgânica e Inorgânica / CENTRO DE CIÊNCIAS / UNIVERSIDADE FEDERAL DO CEARÁ; [4] University of St Andrews; [5] Universidade Federal do Ceará - UFC

- Hierarchical films of bacterial celullose/ Ca2+, Cu2+ e Zn2+ exchanged zeolite A were prepared by casting route.
- Composite films presented high performance on controlled release of NO.

Humidity effect on the butanone sensing performance of hollow ZnO structure

https://proceedings.science/p/120566

Tarcísio Micheli Perfecto [1]; Cecilia de Almeida Zito [1]; Diogo Paschoalini Volanti [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

High performance to detect low concentrations of butanone on volatile phase at dry atmosphere. Effective synthesis method to obtain a hollow ZnO structure.

Hydrothermal synthesis of carbon nanoparticles from glucose and urea

https://proceedings.science/p/119496

Pedro Rafael da Cruz Almeida [1]; Jonatas de Oliveira Souza Silva [1]; Mércia Vieira da Silva Sant'Anna [2]; Eliana Sussuchi [2]

[1] Universidade Federal de Sergipe; [2] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS)

Improved gas-sensing performance of hollow cerium dioxide nanospheres

https://proceedings.science/p/120493

Cecilia de Almeida Zito [1]; Tarcísio Micheli Perfecto [1]; Ann-Christin Dippel [2]; Dorota Koziej [3]; Diogo Paschoalini Volanti [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] DESY; [3] Institute of Nanostructure and Solid State Physics, University of Hamburg

Hollow CeO2 presented higher sensitivity, stability, and faster responses to CO2 than commercial CeO2 nanoparticles. Improvement in the CO2-sensing performance by tuning the morphology of CeO2.

Influência do hidrogel compósito nas características do fruto do meloeiro

https://proceedings.science/p/119843

Ana Karen Melo Castro Farias [1]; Alana A. Lourenço [1]; Maria Sandra B. Souza [1]; Marcio Marcio Facundo Aragão [2]; Luís Gonzaga Pinheiro Neto [2]; Francisco Helder Almeida Rodrigues [1]; Valdelânia R. Nascimento [2]

[1] Universidade Estadual Vale do Acaraú; [2] Instituto Federal de Educação, Ciência e Tecnologia do Ceará

The soil with hydrogel provided better water comfort for the plants and fruit, for the variables analyzed.
Better development of melon fruits using hydrogels.

Influência dos ligantes de superfície em nanocristais de ZrO2 na preparação e propriedades de nanocompósito acetato de celulose:ZrO2

https://proceedings.science/p/120189

Cleocir José Dalmaschio [1]

[1] Universidade Federal do Espírito Santo

Highlights Influence of surface ligands on ZrO2 nanocrystals in the preparation and properties of nanocomposite with cellulose acetate; Functionalization of nanocrystals to control interfacial region between phases; Nanocomposite cellulose acetate membrane; Thermal properties of nanocomposite. **Resumo/ Abstract** Nanocompósitos são materiais que resultam da combinação de dois ou mais materiais em fases distintas, sendo que pelo menos uma das fases se encontre em dimensão nanométrica. Em muitos nanocompósitos as propriedades em aplicação se apresentam superior, quando comparado ao material da matriz individual. Um exemplo de nanocompósito é a combinação envolvendo polímeros e nanocristais inorgânicos, esse tipo de compósito apresenta como uma das vantagens a processabilidade, a qual se mantem da matriz polimérica. Na preparação de nanocompósito de matriz polimérica o sinergismo entre as fases é de extrema relevância sendo que esse sinergismo impacta nas propriedades do material final [1]. Para avaliar o sinergismo e a dispersão de nanocristais inorgânicos funcionalizados com uma matriz de acetato de celulose, foram sintetizadas nanoestruturas de ZrO2 em três diferentes solventes orgânicos [2] os quais foram incorporados na matriz polimérica para obtenção de membranas. Os nanocompósitos obtidos foram

caracterizadas por microscopias e técnicas de análises térmicas. A caracterização por microscopia evidenciou duas características de interação dos nanocristais com o polímero, sendo que os nanocristais funcionalizados com ligante oleato (OAc) resultaram em dispersão mais uniforme, enquanto os ligantes benzoato (BnOH) e octanoato (OcOH) geram a formação de ilhas de nanocristais na matriz, quando na concentração de 20% (m/m) inorgânico/polímero. Uma segunda característica associada ao contraste obtido das imagens de microscopia ótica, indica que o benzoato promove uma melhor interação nas transições entre fases inorgânica/orgânica. Análises termogravimétricas e calorimetria exploratória diferencial indicaram uma elevação nas temperaturas de degradação (Td) - até 17°C - e na temperatura de cristalização (Tc) - até 11°C - no compósito quando comparado ao polímero puro. Tal elevação está associado a redução de mobilidade da cadeia polimérica, pela presença dos nanocristais na matriz.

Iron catalyst obtained from waste cooking oil: Synthesis of carbon material for emerging contaminants removal

https://proceedings.science/p/119554

Michelle Pains Duarte [1]; Ana Paula de Carvalho Teixeira [1]
[1] Universidade Federal de Minas Gerais

Synthesis of carbon material by floating catalyst chemical vapor deposition (FC-CVD) process. Use of iron carboxylates obtained from waste cooking oil as catalyst. Adsorption of emerging contaminants.

Isotherm investigations of the adsorption of Methylene blue from aqueous solutions using chitosan-g-poly(acrylic acid)/poly(acrylamide)

https://proceedings.science/p/120005

Francisco Helder Almeida Rodrigues [1]; Ana Karen Melo Castro Farias [1]; Wescley de Souza Araújo [1]
[1] Universidade Estadual Vale do Acaraú

Highlights The experimental data were better explained by the Langmuir adsorption isotherm. The Langmuir adsorption isotherm suggested a monolayer formation and spontaneous process Abstract In this study, a series of superabsorbent hydrogels based on the biopolymer chitosan (CTS) grafted poly(acrylic acid) or poly(acrylamide) were successfully developed and their ability to adsorb methylene blue (MB) from aqueous solutions was investigated. The adsorption data were fitted with Langmuir and Freundlich isotherm models to understand the interaction mechanisms that take place between the adsorbent and the adsorbate as well as the adsorption process. The isotherm parameters calculated from these models by linear regression method are given in Table 1. Table 1. Langmuir and Freundlich isotherm model parameters for MB adsorption on CTS-g-poly(acrylic acid) and CTS-g-poly(acrylamide) Isotherm Parameters CTS-g-poly(acrylic acid) CTS-g-poly(acrylamide) qe (mg.g-1) 1376 1090 Langmuir qmax (mg.g-1) 1404 1106 kL (L.mg-1) 0,098 0,158 R2 0,99954 0,99986 Freundlich kF ((mg.g-1)(L.mg-1)1/n) 418 423 n 4,57 5,73 1/n 0,21881 0,17452 R2 0,8753 0,7868 The Langmuir isotherm fitted well with the experimental data with R2 values considerably higher than those calculated from the Freundlich isotherm. This data indicates that the adsorption process of MB for both hydrogels is driven by the formation of a dye monolayer on the adsorbent surfaces. In this case, such surfaces show a homogeneous morphology and a finite number of identical sites. Further, the qm,cal values are in agreement with the qe values as demonstrated in Table 1. Other studies using hydrogel for MB removal have found similar behavior1-3. Acknowledgments Acknowledgments: To CNPq, FUNCAP (BP3-0139-00257.01.00/18) and UVA. 1Melo, B.C.; Paulino, F.A.A.; Cardoso, V.A.; Pereira, A.G.B.; Fajardo, A.R.; Rodrigues, F.H.A. Carbohydrate Polymers. 2018, 181, 358. 2Azevedo, A.C.N.; Vaz, M.G.; Pereira, A.G.B.; Farjado, A.R.; Rodrigues, F.H.A. Iranian Polymer Journal. 2017, 26, 93. 3Vaz, M.G.; Pereira, A.G.B.; Farjado, A.R.; Azevedo, A.C.N.; Rodrigues, F.H.A. Water Air Soil Pollut. 2017, 228, 14

Kinetic Study of Fluorescence Quenching of Fluorescein Sodium by Graphene Oxide

https://proceedings.science/p/120633

Danilo Roberto Carvalho Ferreira [1]; Tiago de Mattos Serodre [1]; Estefânia Mara Nascimento Martins [1]; Adelina Pinheiro Santos [1]; Clascidia Aparecida Furtado [1]
[1] CDTN (Centro de Desenvolvimento da Tecnologia Nuclear)

♦Graphene oxide is a super-quencher nanomaterial ♦The quenching process can be dynamic or static with different kinetic parameters ♦Mathematical modeling can distinguish both types each other

Magnetic carbonaceous nanocomposites: preparation and its application as multifunctional adsorbents

https://proceedings.science/p/120242

Lais Helena Sousa Vieira [1]; Carla Manuela Sganzerla Sabino [2]; Francisco Holanda Soares Júnior [3]; Janaina Sobreira Rocha [1]; Manuela Oliveira Castro [4]; Rafael Silva Alencar [5]; Luelc S. Costa [6]; Bartolomeu Cruz Viana Neto [7]; Amauri Jardim de Paula [1]; João Maria Soares [8]; Antonio Gomes Souza Filho [1]; Larissa Otubo [9]; Pierre Basílio Almeida Fechine [10]; Anupma Gosh [1]; Odair Pastor Ferreira [2]

[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Universidade Federal do Ceará, Campus do Pici, Departamento de Física; [3] Instituto Federal de Educação, Ciência e Tecnologia do Ceará; [4] Universidade Estadual do Ceará; [5] Universidade Federal do Pará; [6] Universidade Estadual de Campinas; [7] Universidade Federal do Piauí; [8] Universidade do Estado do Rio Grande do Norte; [9] Instituto de Pesquisas Energéticas e Nucleares / CNEN; [10] Universidade Federal do Ceará, Departamento de Química Analítica e Físico Química

Hydrothermal carbonization followed by thermochemical activation to prepare multifunctional adsorbent; Fe3O4 and Fe0 were the
magnetic phases obtained after the thermochemical activation.

Microwave-assisted synthesis of tungsten-doped bismuth vanadate photocatalysts with controlled morphology

https://proceedings.science/p/120432

Barbara Scola Rodrigues [1]; Carolyne Martins Branco [1]; Juliana dos Santos de Souza [1]

[1] Universidade Federal do ABC

• Optimized microwave-assisted synthesis of (W)BiVO4; • Structural and morphologic effect of using Polyvinylpyrrolidone (PVP); • Enhancement of BiVO4 photocatalytic activity through tungsten-doping.

Multiple approach for the production of nano-hexagonal boron nitride on a larger scale - strategies of a technology center

https://proceedings.science/p/120337

Glaura Goulart Silva [1]

[1] CTNano/UFMG

Nanocomposites of β-cyclodextrin polymers with silver nanoparticles: photocatalysis of methylene blue and catalysis of 4-nitrophenol to 4-aminophenol applications

https://proceedings.science/p/120357

Mariane Silva da Cruz [1]; Tiago Alberto Santos Nunes [1]; Viviane Costa de Souza [1]; Lucas Soares Fernandes [1]; Zaine Teixeira Camargo [1]

[1] Universidade Federal de Sergipe

Studies related to cyclodextrin (CD) polymers have grown in recent years to produce multifunctional materials with minimal environmental impacts. This is associated with the low toxicity of CD polymers as well as their ability to remove pollutants and to stabilize nanoparticles. The objectives of the present work were to evaluate the catalytic activity of a nanocomposite of **β**-CD polymer and silver nanoparticles (AgNP) [2] in the reduction of 4-nitrophenol to 4-aminophenol and to verify the photocatalytic capacity in the removal of organic pollutants, using blue methylene (MB) as a model. The polymer was obtained by esterification of **β**-CD with glutamic acid and was used to obtain AgNP in a single step, as a reducing and stabilizing agent. For the catalysis tests, the catalytic activity of the nanocomposite in the reduction of 4-nitrophenol in the presence of excess sodium borohydride in water was observed under heterogeneous conditions and the UV-vis absorbance spectra were obtained. From the 4-nitrophenol reduction

assays, it was possible to verify the catalytic activity of silver nanoparticles in 16 min, with a significant reduction in absorption at 400 nm indicating the conversion of p-nitrophenol to p-aminophenol. The spectrophotometric tests of the photocatalytic activity using the nanocomposites of an aqueous solution of MB indicated a photodegradation of the dye, as there was a decay of the absorption band at 664 nm. This fact is associated with a reduction in the concentration of the dye chromophore group. The nanocomposites have shown promising results to act in the environmental catalysis.

Nanopartículas de prata suportadas em carvão ativado oriundo de Capim Annoni (Eragrostis plana Nees) para redução catalítica do nitrofenol

https://proceedings.science/p/120362

Williane dos Santos Francisco [1]; Andrei Vallerão Igansi [1]; Caroline Ruas [1]; Tito Cadaval [1]; Flávio André Pavan [2]; Marcos Alexandre Gelesky [1]
[1] Universidade Federal do Rio Grande; [2] Universidade Federal do Pampa

Silver nanoparticles supported active carbon from Capim Annoni (Eragrostis plana Nees) for catalytic reduction of nitrophenol. This nanomaterials may be used for removal pollutants from water.

Novel carbon-carbon composites based on nitrogen-doped carbon nanotubes

https://proceedings.science/p/120331

Simone da Silva Simões [1]; Cristal Martínez Ibañez [1]; Andre Galembeck [1]; Eduardo Henrique Lago Falcão [1]; Fernando Jaime Rodríguez-Macías [2]
[1] Universidade Federal de Pernambuco; [2] Instituto Tecnológico y de Estudios Superiores de Monterrey

Porous carbon-carbon composites were prepared by sol-gel, freeze-drying, and CVD.
Composites can withstand up to 10,000 times their own weight.

Optical and structural study of cerium doped niobium oxides as photocatalysts under solar radiation

https://proceedings.science/p/119539

Bruno Antonio Trajano Menezes [1]; Juliana Fonseca de Lima [1]; Marcos Colaço [1]; Daiane Ribeiro [1]
[1] UNIVERSIDADE DO ESTADO DO RIO DE JANEIRO

Photocatalysis is contextualized in a broad technological development environment, with applications ranging from the degradation of organic substances, sterilization of hospital utensils as an antibacterial agent and energy conversion processes solar cells1 When compared to other countries, Brazil is located in an intertropical zone, having the advantage of receiving high levels of solar radiation throughout the year. Therefore, developing of photocatalysts capable of using energy from the sun is desirable, and doping can cause changes in the range of semiconductor absorption2 The solid materials were synthesized by hydrothermal method employing ammonium niobium oxalate and cerium(III) nitrate as precursors, then the samples were calcined at 800 oC for 5 h. Cerium doped niobium(IV) oxides were characterized about their structure (FTIR, DRX, Raman and XPS), morphological (SEM) and optical (DRS) properties, and photocatalytic activity. [1] KUWAHARA, Yasutaka et al.. Journal of Catalysis v. 285, n. 1, p. 223–234, jan. 2012 [2] GÓMEZ, J.M. Rodríguez et al.. Revista Brasileira de Ensino de Física v. 40, n. 3 , 26 mar. 2018

Optical-vibration properties of Li2ZnGeO4 and Na2ZnGeO4 ortogermanates

https://proceedings.science/p/119771

Jéssica Viegas [1]; Anderson Dias [1]; Rberto Moreira [1]
[1] Universidade Federal de Minas Gerais

Zinc germanates are promising materials for microwave and luminescent applications, such as wireless communication, LEDs and several other electronic devices. In this work, the monoclinic phase (P21/n, # 14) of Li2ZnGeO4 was obtained by conventional solid-state reaction at 1000 °C, for 4 hours, followed by sintering at 1100 °C, also for 4 hours. By its turn, Na2ZnGeO4 was synthesized by conventional solid-state reaction at 900 °C, for 2

hours, and sintered at 1100 °C, for 4 hours. The obtained phase also belongs to a monoclinic structure, with space group Pn (# 7). The vibrational properties of the compounds were evaluated by polarized Raman spectroscopy, which allowed the determination, for the first time, of the vibrational Raman modes for Li2ZnGeO4 and Na2ZnGeO4. Infrared-reflectivity measurements were performed for both sintered compounds, at the medium- and far-infrared regions. By this study, it was possible to observe the most relevant polar modes foreseen by Group Theory analysis and determine the frequencies and damping constants of the transversal and longitudinal branches for these materials, as well as their related dielectric response (e" for TO modes; (1/e)" for LO ones).

PEBA/Hidróxidos Duplos Lamelares como curativos terapêuticos multifuncionais

https://proceedings.science/p/120632

Mariana Pires Figueiredo [1]; Ana Borrego-Sánchez [2]; Fátima García-Villén [2]; César Viseras [2]; Vera Regina L. Constantino [3]

[1] Departament of Fundamental Chemistry, Institute of Chemistry, University of São Paulo ; [2] University of Granada; [3] Departament of Fundamental Chemistry, Institute of Chemistry, University of São Paulo.

Multifunctional polymeric dressings possessing improved mechanical performance, able to sustain and modulate a drug release by the presence of Layered Double Hydroxides drug carriers

Performance of water oxidation by 3D Printed Electrodes modified by Prussian blue analogues

https://proceedings.science/p/119932

Juliano A. Bonacin [1]; Priscilla J. [2]; Amanda T. N. [3]; Rodrigo R. [4]; Gabriel de O. [5]; Andre Formiga [6]

[1] Universidade Estadual de Campinas; [2] Zambiazi; [3] de Moraes; [4] Kogachi; [5] Aparecido; [6] Formiga

The water oxidation is the limiting step in the water-splitting process[1],[2]. Given this scenario, the development of new catalysts is essential in this field. The emergent demanding is the use of Earth-abundant elements and catalysts with high performance under mild condition. Because of this, catalysts such as Prussian Blue analogues have been receiving a lot of attention in recent years[3]. In addition, working under neutral conditions allow us to take advantage of the modification of conductive polymeric 3D printed electrodes with Prussian blue. Thus, we described in this work, the development of the polymeric 3D printed electrodes modified by Cobalt-Prussian blue and their performance in the water oxidation reaction (WOR). [1] Godwin, I.; Rovetta, A.; Lyons, M.; Coleman, J. ;Curr. Opin. Electrochem. 2018, 7, 31 [2] Craig, M. J.; Coulter, G.; Dolan, E.; Soriano-López, J.; Mates-Torres, E.; Schmitt, W.; García-Melchor, M. ;Nat. Commun. 2019, 10, 1 [3] M. Pires, B.; Santos, P. L. dos; Katic, V.; Strohauer, S.; Landers, R.; B. Formiga, A. L.; A. Bonacin, J. ;Dalton Trans. 2019, 48, 4811

PHOTOCATALYSIS OF BLUE ASTRAZON FGGL 300% USING QUANTUM DOTS OF PURE ZnO AND ZnO DOPED WITH Fe(III) FOR DISCOLORATION

https://proceedings.science/p/119748

Lizandra Maria Zimmermann [1]; Samara de Quadros [1]

[1] Universidade Regional de Blumenau

Zinc oxide quantum dots (ZnO) as photocatalyst. Fe(III)-doped ZnO QDs. Photodiscoloration of blue astrazon FGGL 300% (textile effluent) with the use of UV and artificial sunlight.

Poly(butylene adipate-co-terephthalate) (PBAT) antimicrobial film with clove essential oil for use in active packaging

https://proceedings.science/p/119481

Geisse Elike Pereira Amorim [1]; Ivo Diego Lima Silva [2]; Tamires da Silva Lima [2]; Glória Maria Vinhas [2]; Elaine Cristina Lima do Nascimento [1]; Andrea Monteiro Santana Silva Silva Brito [1]

[1] Universidade Federal Rural de Pernambuco - UFRPE; [2] Universidade Federal de Pernambuco - UFPE

The PBAT film added with clove essential oil proved to be promising for use in active packaging; The films presented good visual, physical, chemical and antimicrobial characteristics.

Pontos de carbono luminescentes obtidos a partir da quitosana e suas aplicações como sensores de íons metálicos

https://proceedings.science/p/120429

Alessandra Pires Passos Zattar [1]; Fabiano Vargas Pereira [1]; João Paulo de Mesquita [2]
[1] Universidade Federal de Minas Gerais; [2] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Carbon dots (CDs) were obtained from chitosan.
The CDs presented an average diameter of 2.4 ± 1.2 nm and a quantum yield of 9.3%.
The nanoparticles were used as sensors for different metal ions.

Preparation and characterization of silver nanoparticles/carbon nanocomposites for water purification and disinfection

https://proceedings.science/p/119836

Pedro Miguel Carneiro Jeronimo [1]; Carla Manuela Sganzerla Sabino [1]; Laís Helena e Sousa Vieira [2]; Maria Clara Fernandes de Andrade [1]; Enzo Victorino Hernández Agressott [1]; Alexandre Rocha Paschoal [1]; Francisco Holanda Soares Júnior [3]; Amauri Jardim de Paula [1]; Odair Pastor Ferreira [1]
[1] Universidade Federal do Ceará, Campus do Pici, Departamento de Física; [2] Universidade Federal do Ceará; [3] Instituto Federal de Educação, Ciência e Tecnologia do Ceará, Campus Limoeiro do Norte, Departamento de Ensino

Activated carbon was prepared by thermochemical activation from a hydrothermal carbon (hydrochar). The nanocomposite was obtained by wet impregnation of the activated carbon with silver nanoparticles.

Preparation and colorimetric characterization of patterned plasmonic structures made of nanosilver or nanogold deposited on PDMS parts

https://proceedings.science/p/120007

Elias Santos [1]
[1] Universidade Federal de São Paulo

Preparation of a quaternary nanohybrid material (MWCNTCO-NHCbzNH-COTh-g-rrP3DDT) with electrochromic enhancement

https://proceedings.science/p/120102

Hállen Daniel Rezende Calado [1]; Marcus Henrique de Araujo [1]; Claudio Luis Donnici [1]
[1] UFMG

Since the discovery of the carbon nanotubes (CNT) and their impressive mechanical, electrical, and optical properties, innumerous works have been focused towards the development of approaches to attach several kinds of molecules with multifunctional properties. On another hand, the discovery of the conjugated polymers, like the polythiophenes, was a landmark on researches concerning the development of technological materials with high performance, conductivity, thermal stability, and low costs. On this way, strategies that combine these two individual groups into novel nanohybrid materials have become an astonishing methodology for tailoring and fine-tuning multivariate properties. Herein, we have aimed the preparation of a novel quaternary nanohybrid material based on covalent bonds between oxidized multi-walled carbon nanotubes (MWCNT-ox), 3,6-diamino-9-methylcarbazole (H2NCbzNH2), 3-carboxythiophene (ThCO), and the final grafting of regioregular poly(3-dodecyl thiophene) (rrP3DDT). Indeed, all spectroscopic analysis, specially X-ray photoelectron spectroscopy (XPS), have proved the predicted covalent bonds formation between the units. Through thermogravimetric analysis (TGA) the CNT content was estimated around 50%wt. This nanohybrid has also been characterized by cyclic voltammetry in order to know its electroactivity

window. On the sequence, a solution of this material was casted over an ITO-coated glass to form a thin film, which was submitted to several conditioning potentials, measuring the UV-Vis spectrum for each one. Like expected, the hybrid has presented a reversible color changing going from orange (at reduction potential) into colorless (at oxidizing potential). Moreover, it showed a better electrochromic performance, with a coloration efficiency almost twice higher than pristine P3DDT, fast times of response for coloration/bleaching processes, and greater long-term electrochromic cyclability. Indeed, the electrochromic properties have been enhanced due to the CNT presence beyond the covalent bonds between the units, corroborating once more, the benefits of tailored and designed approaches to achieve electrochromic materials with improved performance.

Produção de Nanotubos de TiO2 por anodização em diferentes tempos utilizando NH4F e glicerina.

https://proceedings.science/p/120597

Victoria Amatheus Maia [1]; Neila Braga [1]
[1] Universidade Federal do Amazonas

In this work, the synthesis of titanium oxide (TiO2) nanotubes by electrochemical anodization were performed by studying effect of time in nanotubes growth. Nanotube were grown in 25V potential in glycerin and 10% DI water + Nh4F 0,06 mol/L using Pt wire (10 mm in front of Ti).

Products and intermediates formed by hydrothermal treatment of Al2O3 in Ni(NO3)2 aqueous solution.

https://proceedings.science/p/120383

Gustavo de Estácio Borges [1]
[1] Universidade Federal de São Paulo

Nickel compounds, such as NiO and Ni/Al2O3, was formed by hydrothermal treatment in low temperature using as reagents alumina and aqueous nickel nitrate. The reaction time, stirring and temperature was investigated.

Propriedades magnéticas de nanomateriais de CeO2 em função de diferentes morfologias: nanofios, nanocintos e nanoesferas.

https://proceedings.science/p/120484

Juliana Pires de Souza [1]; Odivaldo Alves [1]; Júlio César Martins Silva [1]; Jilder P. Serna [2]; Leticia Moraes [3]
[1] Universidade Federal Fluminense; [2] Centro Brasileiro de Pesquisas Físicas; [3] Instituto de Pesquisas Energéticas e Nucleares / CNEN

Ceria nanomaterials are ferromagnetic due to presence of oxygen vacancy and Ce3+ ions. The material's morphology changes the number of vacancies on the surface and influences its magnetic properties.

PVA films with gold nanoparticles: A new method for detecting drugs as possible pollutants.

https://proceedings.science/p/120006

Renan Tostes Couto [1]; Marcelo Victor Cunha do Amaral [1]; Alexandre de Camara [1]; Juliana Fonseca de Lima [1]
[1] UNIVERSIDADE DO ESTADO DO RIO DE JANEIRO

Synthesis and characterization of 8 and 20 nanometers gold nanoparticles;PVA films with gold nanoparticles for sensing captopril in different concentrations Discussion about size influence in sensing

Ruthenium(II) complexes bearing N-heterocyclic-dithiocarbolyxates as new dyes for Organic Solar Cells

https://proceedings.science/p/119543

Murillo da Silva Paiano [1]; Douglas Henrique Nunes Santos [2]; Patrik Dione de Santana Gois [3]; Valdemiro Pereira de Junior [2]

[1] Departamento de Química e Bioquímica / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Departamento de Química e Bioquímica / Faculdade de Ciências e Tecnologia /Universidade Estadual Paulista ; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"

New Ru(II) complexes coordinated with N-heterocyclic dithiocarboxylates were synthesized to act as dyes in Organic Solar Cells (OSCs). This work evaluated systematically different combinations of ancillary ligands in the coordination sphere of the complexes, modulating the spectroscopic and electrochemical properties of these complexes to act efficiently in the processes of electrons transfer involved in these types of solar cells. The whole study extends over three main stages: the initial stage consists in the synthesis of different carbenes N-heterocyclic through a well-known procedure, followed by a direct combination with carbon disulfide obtaining the high-stable zwitterionic dithiocarboxylates ligands. The second stage is the synthesis of Ru(II) complexes coordinated with the planned ligands. The last step, not yet executed, will be directed to the application of these complexes in OSCs for analysis of its photovoltaic efficiency, thermal stability, electronic behavior, and reversibility.

Self-assembled lipopeptides with potential activity against adenocarcinoma cells

https://proceedings.science/p/119799

Karina Brenes [1]; Sandra Valeria Vassiliades [1]; Andrea M. Aguilar [2]; Iseli Lourenço Nantes [1]; Wendel Andrade Alves [1]

[1] Universidade Federal do ABC; [2] Universidade Federal de São Paulo

Self-assembled lipopeptides showed potential antitumor activity against HeLa cells, where peptide aggregation process may is related to cell toxicity.

Shape control of the Cobalt-Prussian blue catalyst and its morphological-dependence on water oxidation reaction

https://proceedings.science/p/119789

Daniel Esteves Bessa Moreira [1]; Thiago de Barros Ferraz [1]; Andre Formiga [1]; Juliano Alves Bonacin [1]

[1] Universidade Estadual de Campinas

Over the past few years, the global energy demand has increased significantly. Fossil fuels are the major source of this energy. However, they have been increasing the number of pollutants in the atmosphere and thus intensifying the greenhouse effect. In this scenario, it is necessary to replace this matrix with technologies that are sustainable. The use of hydrogen (H2) has been highlighted on the world stage because it produces clean energy since the only byproduct of its reaction with oxygen is water. Nevertheless, the majority of hydrogen production (95%) still comes from fossil fuels. One alternative way to produce hydrogen gas is by the water splitting process. However, the water oxidation reaction is the limiting step, once it is kinetically and thermodynamically unfavorable. Thus, the use of catalysts is necessary. Rare metal oxides (RuO2, IrO2) are the state of art for this reaction, nonetheless, their main drawbacks are the high cost and low long-term stability. Cobalt Prussian blue analogues (CoPBA), on the other hand, have received great attention because their kinetics are comparable to state of art catalysts and they are very stable in neutral pH, besides they are easily scalable. In this work, we synthesized a cobalt-Prussian blue catalyst with different morphologies, and we studied its application in the water oxidation reaction. Moreover, we are putting efforts to understand how the morphology affects the catalyst performance. From Scanning Electron Microscopy (SEM), it can be seen different shapes of CoPBA that have been synthesized until now. Electrochemical measurements for water oxidation were also made, as it can be seen in the presentation.

Síntese de eletrodo à base de cobre para oxidação anódica de poluentes em meio aquoso

https://proceedings.science/p/120381

Nathalia Marcelino Pereira Queiroz [1]; Flaviana Freitas Feitosa Ferro [2]; e Carmem Lucia de Paiva Silva Zanta; Josealdo Tonholo [3]

[1] Laboratório de Eletroquímica Aplicada - Universidade Federal de Alagoas; [2] Centro de Tecnologia / Universidade Federal de Alagoas; [3] Universidade Federal de Alagoas

Synthesis of copper-based electrode for anodic oxidation of pollutants in aqueous medium - alternative material for the remediation of wastewater containing resilient, complex and stable pollutants.

Síntese e avaliação anticorrosiva de β-enaminoésteres derivados da anilina halogenada frente ao aço carbono em meio ácido

https://proceedings.science/p/119856

Geicy Kelly Pires Barboza [1]; Mariana Falcão Lopes Princisval Carlos [1]; Aurea Echevarria [1]

[1] Universidade Federal Rural do Rio de Janeiro

Synthesis and anticorrosion evaluation of enaminoesters halogenated aniline derivatives against steel carbon AISI 1020 in acid medium. This work performed the evaluation of theanti-corrosion effect.

Síntese e caracterização de sistema nanocarreador de um sistema composto pelo complexo La(Lapachol)3 e nanopartículas de SiO2 para terapia do câncer

https://proceedings.science/p/120558

Fernanda Timóteo [1]; Juliana Jorge [2]; Marco Antonio Utrera Martines [2]; Adriana Pereira Duarte [2]

[1] Instituto Federal de Educação, Ciência e Tecnologia de Mato Grosso do Sul; [2] Universidade Federal de Mato Grosso do Sul

The main highlight of this work is to use a biocompatible inorganic matrix, silica nanoparticles, as a carrier to a potential anticancer complex La(Lapachol)3.

Síntese e caracterização de TiO2/SnO2 com diferentes teores de Sn e avaliação da atividade fotocatalítica.

https://proceedings.science/p/120274

Igor Matheus de Amorim Silva [1]; Geovânia Cordeiro [1]; Thatiane Veríssimo dos Santos [2]; Mario Roberto Meneghetti [3]; Simoni Margareti Plentz Meneghetti [1]

[1] Universidade Federal de Alagoas, Grupo de Catálise e Reatividade Química e Instituto de Química e Biotecnologia; [2] Universidade Federal de Alagoas, Grupo de catálise e Reatividade Química e Instituto de Química e Biotecnologia.; [3] Universidade Federal de Alagoas

Photocatalytic degradation of methylene blue;
Heterojunctions improve photocatalytic activity.

Síntese e comportamento em água de hidrogéis baseados em Gelatina e Siloxano

https://proceedings.science/p/120271

Lavínia Silva do Nascimento [1]; Lígia Passos Maia-Obi [1]

[1] Universidade Federal do ABC

O colágeno tem atraído interesse como biomaterial devido a sua biocompatibilidade, degradabilidade e, na forma de gelatina, sua capacidade de formar hidrogéis e aerogéis, que podem ser utilizadas como arcabouços para crescimento celular, mediante a reticulação das cadeias peptídicas (ECHALIER et al., 2017). O presente trabalho teve como objetivo obter hidrogéis a partir da reticulação da gelatina pelo 3-glicidoxipropil trimetoxissilano (GPTMS) e a caracterização de seu comportamento em água. Para a síntese, 100 mg de gelatina (10 %m/v) e 12,8 mg de GPTMS eram solubilizados em água e mantidos a 60 °C, sob agitação, por 2h. Os sistemas resultantes tiveram a água removida em estufa (amostra GSH_1) ou por liofilização (amostra GSH_2), sendo o material liofilizado também levado à estufa por 48 h, resultando

respectivamente em filmes mecanicamente resistentes e em criogéis porosos. Ambas as amostras ficaram imersas em água e em seguida secas em estufa, para remoção de moléculas que não tenham participado da reticulação, sendo verificado que a %gel (porcentagem de gel) dos materiais foram respectivamente 91 e 99%. Os materiais obtidos foram estudados quando a sua solubilidade em água a temperatura ambiente, durante 6h, sua absorção de água a temperatura ambiente, por 48 h, e sua estabilidade à hidrólise em água a 60 °C, por 10 dias. Foi verificado que as duas estratégias de síntese promoveram reticulações muito eficientes, dado as altas %gel. Foi verificado que os materiais obtidos absorviam grande quantidade de água, sem se solubilizar, caracterizando a formação de hidrogéis, além disso eles mantiveram a sua integridade física durante a absorção de água. Verificou-se ainda que ambas as amostram apresentaram altos teores de absorção, sendo que a GSH_1 teve a sua absorção estabilizada em torno de 200% em massa, enquanto o GSH_2 apresentou um aumento da massa que atingiu 331%, sem haver estabilização de sua massa, indicando possibilidade de maior absorção para tempos maiores de imersão. Este comportamento de absorção pode ser entendido através da morfologia dos materiais. Criogéis apresentam microporos que permitem que além de serem entumescidos, tendo a água ocupando os interstícios na rede do hidrogel, ainda retenham água adicional nestes poros. O teste de estabilidade à hidrólise revelou que ambos os materiais não apresentaram quebra de ligações que levassem à sua erosão ou solubilização. Embora possuam ligações hidrolisáveis Si-O-Si, responsáveis pela reticulação (LEE; KIM; JEONG, 2019) (SEGURA et al., 2017), os materiais se mostraram estáveis em água. Neste trabalho, foi possível reticular a gelatina utilizando o GPTMS e formar hidrogéis com diferentes morfologias, que podem ser utilizadas para modular a absorção de água dos materiais. Além disso os materiais se mostram promissores para a aplicação em biomateriais que não se degradem em água com facilidade. ECHALIER, Cécile et al., Materials Today, [s.l.], v. 20, n. 2, p.59-66, 2017. LEE, Ho-yong; KIM, Hyoun-ee; JEONG, Seol-ha., Colloids and Surfaces B: Biointerfaces, [s.l.], v. 174, p.308-315, 2019. SEGURA, D. L. N. et al.,Verano de la Investigación Científica, v. 3, n. 2, p. 601–605, 2017.

Síntese, caracterização e avaliação de propriedades magnéticas e catalíticas de nanopartículas de níquel-platina frente a eletro-oxidação da ureia

https://proceedings.science/p/120482

Eduardo Magalhães Rodrigues [1]; Jilder P. Serna [2]; Odivaldo Alves [3]; Júlio César Martins Silva [3]
[1] Instituto de Química / Universidade Federal Fluminense; [2] Centro Brasileiro de Pesquisas Físicas; [3] Universidade Federal Fluminense

Ni nanoparticles with small amount of Pt dispersed on the catalysts; Modification of the magnetic properties of nickel caused by platinum; High catalytic activity of NiPt/C for urea electrooxidation.

Solvent Effect on Spectroscopic Properties of Carbon Nanodots

https://proceedings.science/p/120485

Raphael Freire da Silva [1]; Albina Mikhraliieva [1]; Volodymyr Zaitsev [1]
[1] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio)

One-step synthesis by solvothermal method of Carbon Dots (CDs) is prepared, its emission spectra was sensitive to solvent polarity. Bathochromic shift of CDs was observed at changing solvents.

Solvothermal synthesis of MOF 235 and its photoelectrochemical properties under ultraviolet light

https://proceedings.science/p/119434

Luan Pereira Camargo [1]; Adriana Campano Lucilha [1]; Paulo Rogerio Catarini da Silva [1]; Luiz Henrique Dallantonia [2]
[1] Universidade Estadual de Londrina; [2] Departamento de Química / Centro de Ciências Exatas / Universidade Estadual de Londrina

MOF 235 was easily synthetized by solvothermal method. Its present very good electrochemical properties showing a high photocurrent under UV light and excellent photoelectrocatalytic activity.

Spray-dried microspheres of starch and micronutrients as enhanced efficiency fertilizer

https://proceedings.science/p/119731

Camila Gruber Chiaregato [1]; Roselena Faez [2]
[1] Universidade de São Paulo (USP/FZEA); [2] Universidade Federal de São Carlos (UFSCar-Araras)

The agriculture has the challenge to establish strategies to achieve sustainable production of food. Fertilizers are used to increase crop production by replacing the necessary nutrient and also are the major cause of contamination of underground water and rivers. The big question is how to increase fertilizer efficiency and crop yield without compromising natural resources? One of the answers is developing a material that enhance the fertilizer efficiency, reducing the loss, the amount of fertilizer applied and, consequently, production costs. For this purpose, the aim of this work was to develop microspheres of starch and micronutrients (Fe2+, Cu2+ and Mn2+) by spray drying technique. First, we carried out the gelatinization of starch (conditions: oil bath with magnetic stirring, 97 °C, 30 min). After, monoelementary dispersions of starch/micronutrients were done by adding the micronutrients separately and homogenized in a Turrax for 5 min with 10,000 rpm and during the atomization process kept in magnetic stirring. For starch/micronutrient atomization, we use a 2 - fluid nozzle (0.5 mm diameter) at 130 °C and aspiration rate of 10 % in a Mini spray dryer (B290/Buchi), Figure 1 (A). The yield was 44.51, 39.54 and 47.85 % for Starch-Cu, Starch-Fe, and Starch-Mn, respectively. For the release teste, microspheres of starch/micro (0.5 g) were conditioned in a semi-permeable sachet of TNT and immersed in 50 mL of distilled water. At pre-established times, the sachet containing the material was removed and immersed in a new recipient containing the same volume of distilled water. The released micronutrients were quantified by Atomic Absorption Spectrometry. During the 8 days of the test, the release profile was similar for the microspheres containing different micronutrients. The microspheres release 60 % of the nutrients in 60 min, following the increasing order Fe2+<Mn2+<Cu2+, 56, 58 and 64% released, respectively. In 8 days, the increasing order of release became Mn2+<Fe2+<Cu2+, 74, 85 and 86%, respectively, Figure 1 (B). FTIR analyses corroborate the micronutrient release profile, where the Fe2+ and Mn2+ micronutrients have stronger interaction (more intense the shift of the OH bond to higher wavelength), slower release, and Cu2+, weaker interaction (less intense the shift of the OH bond to higher wavelength), faster release in water. It was possible to establish that the release profile of micronutrients in water is related to the interaction force between the inorganic salt cation and the –OH groups of starch. The interaction was more intense for Fe2+ and Mn2+ cations, prolonging the release and less intense for Cu2+, promoting a faster release in water.

Structural and Photophysical Properties of Lanthanide Coordination Frameworks with Pentafluorobenzoate

https://proceedings.science/p/119883

Viviane Pereira de Souza [1]; Rodolfo R. Nunes da Silva [1]; Ivani Malvestiti [1]; Ricardo Luiz Longo [1]
[1] UFPE

Trivalent lanthanide Ln3+ ions have unique photophysical properties and their organic frameworks (LnMOFs) are relevant for many applications. These and other properties are dependent upon the interactions between the Ln3+ ions, which are ubiquitous in LnMOF. Therefore, they are interesting platforms to study these interactions. Pentafluorobenzoic acid (LH) is a strong acid (pKa = 1.48) that can yield coordination compounds (mono and dinuclear and MOFs) with Ln3+ ions. Open synthesis at room-temperature and at 80 °C and liquid-assisted gridding (LAG) mechanochemical method were employed to synthesize the dimer [Ln2(L)6(H2O)8](H2O)2 (Ln = Eu, Gd, Tb) that is already described as well as a new mixed Eu-GdMOF [Ln(L)2(LH)(H2O)4](Cl)(LH)(H2O)2. It structure, determined by crystallography, is quite unusual, because the Ln centers are connected by a single symmetric bridge ligand and a Ln-Ln distance of 6.865 Å, which has not been observed in frameworks of lanthanide-benzoates. The crystal asymmetric unit does not possess an inversion center, however, the crystal packing composed of four asymmetric units does present a center of inversion. Upon excitation at wavelengths larger than 277 nm, the emission intensity of the 5D0 → 7F2 transition in the EuMOF is less intense than the 5D0 →7F1, transition suggesting the presence of an inversion center. However, for the heteronuclear Eu-GdMOF presents the typical 5D0 → 7FJ (J = 0 - 4) transitions, with 5D0 → 7F2 being more intense than 5D0 →7F1. These changes in the relative intensities suggest that (i) the Eu-GdMOF was obtained and the inversion center in the unit cell is no longer present because the replacement of Eu3+ by Gd3+, and (ii) the interactions between the Eu3+ ions are sufficiently strong for the four asymmetric units to behave as a single effective emission center. In the mixed Eu-TbMOF, the typical 5D0 → 7FJ (J = 0 - 4) transitions of Eu3+ and 5D4 → 7FJ (J = 6 - 1) of Tb3+ were observed upon excitation at the ligand states. The excitation spectra present a band due to the 7F6 → 5D4 Tb3+ transition when the emission were monitored at 5D0 → 7F2 or at 5D4 → 7F5, indicating energy transfer from Tb3+ to Eu3+ ions. The reverse energy transfer Eu3+ → Tb3+ was not observed either in the emission or the excitation spectra. The X-ray data as well as the luminescence results showed that the structure of the coordination compounds (dinuclear and MOF) depends on the synthetic method, that the Eu3+ ions interact strongly

even at distances of ca. 7 Å, and that Tb3+ transfer energy to Eu3+ ions. In addition to the novelty of the LnMOF and mixed LnLn'MOFs, their photophysical properties are being explored in several applications.

Study of the colloidal properties of nanofluids containing surface-modified TiO2 nanoparticles with aminosilane

https://proceedings.science/p/119931

Aline Ingrid Alves dos Reis Almeida [1]
[1] UFMG

Gostaria de alterar o título do trabalho para: Surface treatment of TiO2 with 3-aminopropyltriethoxysilane (APTES)

Supporting the Photocatalysts on commercial oxide: An Effective Way to Enhance the Photocatalytic Activity of SrSnO3

https://proceedings.science/p/119507

Ieda Maria Garcia dos Santos [1]
[1] Núcleo de Pesquisa e Extensão/ Laboratório de Combustíveis e Materiais, UFPB

Photocatalysts based on SrSnO3 and SrSnO3@ZrO2 were prepared by the modified-Pechini method at 800°C and applied in the photocatalytic degradation of Remazol Golden Yellow dye under UV radiation. The photohydroxylation of terephthalic acid and scavengers were employed in order to evaluate the participation of each active species, such as hydroxyl radical, and photogenerated electrons and holes on the photocatalytic process. The band gap structure was evaluated using the Mott Schottky method in combination with UV-visible spectrophotometry. According to the results of transmission electronic microscopy (TEM) and X-ray photoelectron spectroscopy (XPS), nanometric SrSnO3 particles were obtained when supported on ZrO2, associated to an increased amount of Sn(II). Results indicated that both samples had high photocatalytic activity, although SrSnO3@ZrO2 showed the best decolorization performance ranging from 32% to 98%, which was associated to the morphology of the particles and to the greater amount of oxygen vacancies. The participation of hydroxyl radicals in the reaction was confirmed when terephthalic acid was used as probe and by using isopropanol as hydroxyl radical scavenger, which resulted in the inhibition of the photocatalytic process. The photocatalytic activity was clearly related to surface redox reactions (Figure 1), as H2O oxidation, with different behaviors in relation to O2 reduction depending on the pH of the solution.

Synthesis and application of composites based on metal sulfides, carbon structures in high performace supercapacitors.

https://proceedings.science/p/119633

Rubens Lucas de Freitas Filho [1]; Renata Figueredo Martins [1]; Túlio Matencio [1]; Arilza de Oliveira Porto [1]; Ana Paula de Carvalho Teixeira [2]
[1] Departamento de Química / Instituto de Ciências Exatas / Universidade Federal de Minas Gerais; [2] Universidade Federal de Minas Gerais

Synthesis of binary and ternary composites with graphene oxide, metal sulfides and helical carbon nanotubes. Applicattionas electrodes for supercapacitors.

Synthesis and characterization of adsorbents for adsorption of contaminants

https://proceedings.science/p/120282

Nelcy Della Santina Mohallem [1]
[1] UFMG

SYNTHESIS AND CHARACTERIZATION OF CARBON DOTS SUPPORTED IN REDUCED GRAPHENE OXIDE.

https://proceedings.science/p/119564

José Carlos dos Santos Junior [1]; Jonatas de Oliveira Souza Silva [1]; Eliana Sussuchi [2]; Marcelo Oliveira Rodrigues [3]
[1] Universidade Federal de Sergipe; [2] Programa de Pós-Graduação em Química (PPGQ)/ Universidade Federal de Sergipe (UFS); [3] Universidade de Brasília

Hybrid material based on reduced graphene oxide/carbon dots as modifying on carbon paste electrode. Highly luminescent carbon dots.

Synthesis and Characterization of Heterostructures Based on Sulphur Doped Polymeric Carbon Nitride (PCN) and Gold Nanoparticles (NPs)

https://proceedings.science/p/119584

Ingrid Fernandes Silva [1]; Ivo F. Teixeira [2]; Ana Paula de Carvalho Teixeira [1]; Humberto Osório Stumpf [1]
[1] Universidade Federal de Minas Gerais; [2] Universidade Federal de São Carlos

PCNs are polymeric semiconductor materials, which have moderate bandgap values, around 2.7 eV, making them active photocatalysts in the UV-Vis region for a series of reactions. The heterostructures based on PCNs and Au NPs have been widely studied in photocatalysts, because of the unique characteristics that arise from the synergism between them, which occur as a result of the excitation of gold by Localized Surface Plasmons Resonance (LSPR). In order to enhance the photocatalyst properties of sulfur doped PCNs and investigate the synergistic effect with Au NPs, four materials with Au NPs of different sizes and shapes were synthesized. These heterostructures were completely characterized by atomic absorption (AA), TEM, XRD and diffuse reflectance in the UV-vis region. The XRD for the synthesized materials displayed peaks characteristic for gold cubic structures. TEM images show that Au NPs and Au nanorods (NRs) are, in general, well dispersed in the material. In addition, bandgap values for composites have decreased compared to pure PCN. Then, the Au NPs and Au NRs increase the photocatalytic activities of the materials and give hybrid photocatalysts a wide range of absorption of light. Highlights

- Active polymeric semiconductors in the UV-Vis region.
- Synthesis of four new hybrid heterostructures based on PCN with gold NPs in their structures.
- Tuning of the electronic properties of PCN.

Synthesis and characterization of morphology-controllable of ZnO nanoparticles and performance evaluation of photocatalysis degradation.

https://proceedings.science/p/120000

Maria Laura Della Costa [1]; Nathália Rodrigues da Silva [2]; Aroldo Geraldo Magdalena [2]; David Padovini do Santos Souza [2]; Fenelon Martinho Lima Pontes [2]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"

A contaminação do meio ambiente por elementos tóxicos, devido à crescente ação antrópica, tem afetado diretamente o equilíbrio ambiental. As nanopartículas de ZnO, com características não tóxicas, baixo custo e alta disponibilidade, têm sido reconhecidas como um material de propriedade fotocatalítica expressiva, sendo uma ferramenta versátil para a remediação ambiental. Nanopartículas de ZnO podem apresentar diversas morfologias, que estão diretamente ligadas a atividade fotocatalítica, e podem ser estudadas e controladas através da síntese. O presente trabalho avaliou a síntese, caracterização e estudo da superfície das nanopartículas de ZnO, as quais foram realizadas pelo método de co-precipitação, utilizando dois agentes precipitantes para estudo (NaOH e NH4OH). Através do DRX foi possível constatar a formação de ZnO, com parâmetros de difração similares para as amostras em análise. Imagens (MEV) revelaram a alteração da morfologia dependo do agente precipitante, sendo observado morfologia tipo wires/espiga de milho para NaOH e esférica para NH4OH. Avaliações de eficiência fotocatalítica na degradação de Rodamina B, foram realizadas em um reator com lâmpada UV 26w, na presença de 50 mg do material e 10 ml do corante à 10 ppm, pH 6, por 180 minutos. À vista disso, foi possível compreender que morfologia tipo esférica aprimoram a fotocatalização, atingindo melhor eficiência em menor tempo, todavia, ambas são eficientes para o processo, apontando uma taxa de degradação máxima muito próxima à 100%.

SYNTHESIS AND CHARACTERIZATION OF ZEOLITE LTA ENCAPSULATED IN CALCIUM ALGINATE FOR TOXIC METALS REMOVAL FROM AQUEOUS MEDIA

https://proceedings.science/p/119947

Antônia França [1]; Conceição Alves [2]; Edmilson de Sousa Almeida [1]; Silvio Oliveira [1]; Ronaldo Ferreira do Nascimento [3]; Adonay Loiola [1]

[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Departamento de Química Orgânica e Inorgânica / Centro de Ciências / UNIVERSIDADE FEDERAL DO CEARÁ; [3] Departamento de Química Analítica e Físico-Química / CENTRO DE CIÊNCIAS / UNIVERSIDADE FEDERAL DO CEARÁ

Hierarchization of zeolite LTA with calcium alginate. FTIR, XRD, SEM characterization. Efficient adsorption of toxic metals by hierarchical zeolite.

Synthesis and photophysical properties of core@multishell NaYF4:Yb,Er@NaYF4:Nd@SiO2 upconversion nanoparticles

https://proceedings.science/p/120033

Gesiane Pinha de Sousa [1]; Fernando Aparecido Sigoli [1]; Italo Odone Mazali [1]

[1] Universidade Estadual de Campinas

Upconversion nanoparticles hierarchically organized in a core multi-shell structure, ß-NaYF4:Er,Yb@NaYF4:Nd@SiO2. Evaluation of different methods for the synthesis of a thin silica shell.

Synthesis of AuNP@PEDOT Composite for Application on Biological Systems

https://proceedings.science/p/119898

Beatriz de Andrade de Faria [1]

[1] Instituto de Química - USP

Synthesis of bimetallic plasmonic nanoparticles for dye photodegradation

https://proceedings.science/p/119814

Rhauane Almeida Galvao [1]; Emanuely José [2]; Larissa Agostinho de Santa Cruz Oliveira [1]; Giovanna Machado [3]

[1] Universidade Federal de Pernambuco - UFPE; [2] UNIVERSIDADE DE PERNAMBUCO; [3] Centro de Tecnologias Estratégicas do Nordeste

Bimetallic plasmonic nanoparticles are suitable for visible light absorption. They can interact with sunlight and generate charge carriers to conduct reactions, for example, dye degradation.

Synthesis of core-shell Au nanorods@Gd2O3:Er,Yb@Gd2O3:Nd for biomedical applications

https://proceedings.science/p/119773

Edison Huertas Montoya [1]; Italo Odone Mazali [1]; Fernando Aparecido Sigoli [1]; Flávia de Sousa [1]

[1] Universidade Estadual de Campinas

Synthesis of geopolymers using CTAB as a structure-directing agent and their use as Amoxicillin adsorption agents

https://proceedings.science/p/119567

Ana Luisa Abrantes Simões [1]; Sara Silveira Vieira [1]; Maria Helena Araujo [1]

[1] Universidade Federal de Minas Gerais

Synthesis of geopolymers using kaolinite and metakaolin as precursors and CTAB as a structure-directing agent. Geopolymers present excellent Amoxicillin adsorption percentages in general.

Synthesis of pyrimidinium-N-heterocyclic-dithiocarboxylates coordinated to Ruthenium(II) complexes and their application in Organic Solar Cells

https://proceedings.science/p/119489

Douglas Henrique Nunes Santos [1]; Murillo da Silva Paiano [1]; Valdemiro Pereira de Junior [1]
[1] Departamento de Química e Bioquímica / Faculdade de Ciências e Tecnologia / Universidade Estadual Paulista "Júlio de Mesquita Filho"

The influence of the divalent cation on the structural and luminescent properties of the MY2O4:Eu3+(M = Ba2+orSr2+) red-emitting phosphor

https://proceedings.science/p/119878

Leonardo Figueiredo Saraiva [1]; Bárbara Sprocati [1]; Airton Bispo [1]; Sergio A Marques de Lima [2]; Ana Maria Pires [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista-Unesp

The Pechini's modified method of two different red-emitting phosphors (BaY2O4:Eu3+ or SrY2O4:Eu3+) with the same crystalline structure led to different phase-purity and luminescent properties.

Thermal and structural characterization of the natural fiber from rubberwood

https://proceedings.science/p/120560

Maycon Jhony Silva [1]; Yasmin da S. Sampaio [2]; Elaine C. P. Gonçalves [3]; Maria Alice Martins [4]; Luiz Henrique Capparelli Mattoso [4]
[1] Programa de Pós-Graduação em Química / Universidade Federal de São Carlos; [2] Universidade Federal de São Carlos; [3] Agência Paulista de Tecnologia dos Agronegócios, APTA-Colina; [4] Bolsista produtividade CNPq / EMBRAPA

Evaluation of natural fiber from rubber tree for to production of composites and nanocomposites. Reuse of agro industrial waste. Value aggregation to the rubber production chain.

Use of graphene oxide and zeolite A in thin-film composite membranes for water desalination processes

https://proceedings.science/p/120582

Robson de Almeida [1]; Juliana Izidoro [2]; Denise Fungaro [2]; Jairo Pedrotti [3]
[1] PPGEMN / Escola de Engenharia / Universidade Presbiteriana Mackenzie; [2] Instituto de Pesquisas Energéticas e Nucleares / CNEN; [3] Universidade Presbiteriana Mackenzie

- Desalination capacity of thin-film composite membranes with graphene oxide and zeolite A. - Removal of sodium, calcium, and magnesium ions by the filtration process.

Use of Rhodamine B in spray-dried PVA/Starch microcapsules to evaluate the encapsulation

https://proceedings.science/p/119676

Felipe Bernegossi Villa [1]; Camila Gruber Chiaregato [2]; Roselena Faez [1]
[1] Universidade Federal de São Carlos; [2] Universidade de São Paulo (USP/FZEA)

The development of enhanced efficiency release materials has been widely used for several purposes, such as in agriculture, improving the release of nutrients to the soil. This work suggests the formation of microcapsules of starch, a low cost, environmentally friendly biopolymer coated with poly (vinyl alcohol) (PVA), a polymer that shows high potential for biodegradation in a presence of starch. The microcapsules were produced by the spray drying technique using a 3-fluid nozzle (3FN), where the inner and outer layers are composed of starch and PVA, respectively. The Rhodamine B (RB) dye was used with starch to evaluate the microcapsule formation. We used a 2-fluid nozzle (2FN) to compare microspheres and microcapsules structures (Figure 1). PVA solutions were prepared at 3 and 6% (m/v) and dispersions of gelatinized starch 3% (m/v), with the addition of 4% (v/v) of RB 0.2% in the starch. The material was dried under fixed temperature and suction conditions (130°C/100%) with the internal flow of 1.2 mLmin−1 and the external flow of 4.4 mLmin−1 for 3FN and a flow of 4.4 mLmin−1 for 2FN. The materials were characterized by the

release of the dye in the water medium; 0.1 g of the microcapsules/microspheres were conditioned in a TNT sachet and placed in 50 mL of deionized water. The water was changed after a certain time. The RB was quantified by the UV-Vis technique (554 nm). The microspheres showed a release of 84.5% in 360 min, while microcapsules, which were covered by an extra layer of PVA, released 81.1% and 82,7% at the same time (Figure 2). Although not expressive, the results show that the materials produced by 3FN had a slower release than the material produced by 2FN, making it possible to optimize and use as strategy to evaluate the active encapsulation.

Química Inorgânica - INO

A new Cu(II) oxamate complex derived from diaminoacridine: Synthesis, caracterization and its catalytic performance towards phenolic compounds oxidation

https://proceedings.science/p/119494

Maria Clara Orioli Emidio Souza [1]; Lucas Hoffmann Greghi Kalinke [2]; Pedro Victor Valadares Romanholo [1]; Lívia Flório Sgobbi [1]; Danielle Cangussu de Castro Gomes [1]
[1] Universidade Federal de Goiás; [2] Instituto Federal de Goiás - Câmpus Anápolis

Synthesis and characterization of the dinuclear Cu(II) complex of formula Na4[Cu2(acriba)2].14H2O, spectroscopic studies of catalytic oxidation of phenolic compounds

A pH dependence of the redox potential of the extremophilic Hell's Gate Globin I (HGbI)

https://proceedings.science/p/120163

Luiz Henrique da Costa Souza [1]; Giamwemberg de Almeida Barreto [2]; Wellinson Gadelha Guimarães [2]; Sueslley Rodrigues [2]; Bruna Talia dos Santos Carvalho [2]; Eduardo Henrique Silva de Sousa [2]; Tércio de Freitas Paulo [2]; Izaura Cirino Nogueira Diogenes [2]
[1] UFC (Universidade Federal do Ceará); [2] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica
Hell's Gate Globin I, a hemeprotein of the Methylacidiphilum infernorum microorganism, was isolated and purified. The dependence of the redox potentials of HGbI on pH results in a pKa value of 6.9.

A study of Pure Cu and Ag/Cu alloy nanoparticles as potential sensor components for optical fiber sensing

https://proceedings.science/p/119700

Marcelo Victor Cunha do Amaral [1]; Renan Tostes Couto [1]; Zeila Virginia Torres Santos [2]; Juliana Fonseca de Lima [1]; Alexandre de Camara [1]
[1] UNIVERSIDADE DO ESTADO DO RIO DE JANEIRO; [2] UCH - Universidad de Ciencias y Humanidades
Synthesis and characterization of pure copper and silver-copper alloy nanoparticles, Discussion about the quality of the produced nanoparticles regarding the synthetic route , the importance of the stabilizing agent during synthesis and the possible usage of those nanoparticles as sensor components in optical sensing.

Ability of Ru-nitrosyl complex to inhibit tumor cell migration through metalloshield of glycosaminoglycans (GAGs)

https://proceedings.science/p/120671

Rafaella Rebecchi Rios [1]; Nicholas Farrell [2]; Roberto Silva [1]
[1] Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), Universidade de São Paulo (USP); [2] Virginia Commonwealth University

The present study shows the ability of Ru-nitrosyl compounds to bind glycosaminoglycans (GAGs) leading to an inhibition of tumor cells migration.

Adsorption and photodegradation of methylene blue using magnetic composites prepared by the combustion methodAdsorption and photodegradation of methylene blue using magnetic composites prepared by the combustion method

https://proceedings.science/p/119604

Matheus Gomes Ferreira [1]; Francisco Garrido [1]; Marta Eloisa Medeiros [1]
[1] Universidade Federal do Rio de Janeiro

Magnetic composites containing ZnO,ZnFe2O4 and VulcanX were prepared by combustion synthesis.These materials have adsorption and photocatalytic properties and can be used to remove dyes from solution.

Análise por EDXRF de pergaminho do século XVIII: ferramenta para a conservação e restauração do documento

https://proceedings.science/p/120524

Mônica Grôppo Parma [1]; Isolda Mendes [2]; Heloisa de Oliveira Beraldo [2]
[1] Departamento de Química / Instituto de Ciências Exatas / Universidade Federal de Minas Gerais; [2] Departamento de Química / Instituto de Ciências Exatas / Universidade Federal de Minas Gerais
Identification of Cu and Zn in gilding. Comparison between the scientific analyses and historical painting treaties.

Analysis of the β-TCP structure obtained from dolomite using the Rietveld Method combined with the Maximum Entropy Method

https://proceedings.science/p/120074

Christiane Philippini Ferreira Borges [1]; Emerson Luiz dos Santos Veiga [1]; Marília Bessa Barros Ferreira [1]; Edson Cezar Grzebielucka [1]; Eder Carlos Ferreira de Souza [1]; André Vitor Chaves de Andrade [1]; Sandra Regina Masetto Antunes [1]
[1] Universidade Estadual de Ponta Grossa
β -TCP (β-Ca3(PO4)2) is a rare naturally occurring mineral, yet it is the second most abundant mineral in bones. By supporting magnesium ion in its structure, when obtained by synthesis, it mimics its natural form. Therefore, it can be used as a material for medical and dental applications, since magnesium promotes better cell adhesion to bone substrate. This study aimed to obtain the β-TCP/Mg2+ phase from dolomite through acid dissolution and precipitation reactions, as well as to investigate the structural changes caused by the addition of magnesium in the β-TCP phase. The β-TCP/Mg2+ synthesis was effective in the production of a potential biomaterial based on calcium phosphates with magnesium in its structure. Rietveld's analyses enabled the identification of two phosphate-rich phases, Ca7Mg9(Ca,Mg)2(PO4)12 and Ca2.66Mg0.34(PO4)2, with β -TCP obtained as the majority phase. It was also possible to observe, by obtaining high-resolution electronic density maps, changes in the β-TCP phase structure caused by the replacement of the magnesium atom in the Ca5 crystallographic site along with possible substitutions to a lesser extent in the remaining calcium sites. The material obtained can have a potential use as biomaterial.

Anthraquinone-Based Linkers for Construction of Stimuli-Responsive Coordination Frameworks

https://proceedings.science/p/120173

João Guilherme Machado de Carvalho [1]; Roland A. Fischer [1]; Alexander Pöthig [1]
[1] Technical University of Munich (TUM)

Three novel anthraquinone-based MOFs were synthesized and structurally characterized. The oxidation state can be modulated in situ. Swichtable features in the solid-state were investigated.

Antitumoral activity of water soluble copper(II) complexes with diamino units against five human tumoral cell lines

https://proceedings.science/p/120421

Wagner da Silva Terra [1]; Érika Soares Bull [1]; Samila R. Morcelli [2]; Rafaela O. Moreira [3]; Leide Laura F. Maciel [4]; João Carlos de A. Almeida [4]; Milton M. Kanashiro [4]; Christiane Fernandes Horn [5]; Adolfo Horn Junior [5]

[1] Instituto Federal Fluminense; [2] Secretaria de Educação do Estado do Espírito Santo (SEDU); [3] Centro Federal de Educação Tecnológica Celso Suchow da Fonseca; [4] Universidade Estadual do Norte Fluminense Darcy Ribeiro; [5] Universidade Federal de Santa Catarina

The cytotoxicity against five human tumoral cell lines (THP-1, U937, Molt-4, Colo-205 and NCI-H460) of three water soluble copper(II) compounds with tetradentade ligands are reported in this work.

Aplicação de um Novo Complexo de Ru(II) contendo um Ligante Heterocíclico Plano Multifuncional

https://proceedings.science/p/119754

Dayane Pedro do Nascimento [1]; Fabio da Silva Miranda [1]

[1] Universidade Federal Fluminense

Application of a new Ru(II) complex containing a planar multifunctional heterocyclic ligand.
Intercalation study of the of a Ru(II) polypyridine complex with DNA.

Application of ZnII and CdII aroilbis(thioureas) complexes for hydrogen production

https://proceedings.science/p/119605

Vânia Denise Schwade

Avaliação da formação do complexo Cu(II)-Carbendazim em águas naturais por medidas eletroanalíticas

https://proceedings.science/p/120157

Eliana Maíra Agostini Valle [1]; CODOGNOTO, L. [1]; Fábio Ruiz Simões [2]; Carolina Zeni Pires Mecca [1]; Ana Layla Carvalho de Lima [1]; Aymara da Silva Santos [1]

[1] UNIFESP - campus Diadema; [2] UNIFESP - campus Baixada Santista

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Avaliação Estrutural e Espectroscópico do tris(n-propilxantato)cobalto(III)

https://proceedings.science/p/120683

Ludmila Cristine Abreu de Azeredo [1]; VICTOR HUGO MALAMACE DA SILVA [2]; Sergio de Paula Machado [1]; Gláucio Braga Ferreira [2]; Marcelo Monteiro Marques [3]

[1] Universidade Federal do Rio de Janeiro; [2] Universidade Federal Fluminense; [3] Coluni- Colégio Universitário Geraldo Reis, UFF

This work has the purpose to report an experimental theoretical spectroscopic study of the complex [(S2COC3H7)3Co] associated with a new characterization by single crystal X-ray.

Binuclear copper(II) complexes with ON chelated phenoxy/naphthoxy–imine ligands: synthesis, characterization, antioxidant activity and cytotoxicity

https://proceedings.science/p/120678

Danielle Tapia Bueno [1]; Adriana Castro Pinheiro [1]; Ianka Jacondino Nunes [1]; Tamara dos Santos Machado [1]; Carolina Cristóvão Martins [1]; Franciele Faccio Bussato [2]; Roberta Cargnelutti [3]; Cristiane Luchese [1]; Osvaldo Casagrande Jr. [4]; Jenifer Saffi [2]; Ethel Wilhelm [1]

[1] Universidade Federal de Pelotas; [2] Universidade Federal de Ciências da Saúde de Porto Alegre; [3] Universidade Federal de Santa Maria; [4] Universidade Federal do Rio Grande do Sul

New binuclear Cu(II) Schiff base complexes were synthesized and characterized. The copper complexes exhibit antioxidant activity and showed low cytotoxicity in mammalian cells.

Bioacelaradores inorgânicos na produção de fertilizante orgânico composto

https://proceedings.science/p/119901

Veronica Machado Mattos [1]; Zenis Novais da Rocha [1]; Jose Petronilio Lopes Cedraz [1]; Suian Lino Oliveira [1]; Neiva Nascimento da Silva [1]; Albert Gonçalves de Sá [1]; Jullietty Cardoso da Silva [1]; Larissa Oliveira Araujo da Silva [1]

[1] Universidade Federal da Bahia

Inorganic bioaccelerators in organic compound fertilizer manufacturing. The stabilization of green coconut shell residue through an inorganic oxidative process.

Captura de CO2 em misturas de glicerol e bases nitrogenadas

https://proceedings.science/p/120245

Isabelle Oliveira Furtado [1]; Thiago Custódio dos Santos [1]; Rodolfo Goetze Fiorot [2]; Larissa Ferreira Vasconcelos [1]; Luciano Tavares Costa [1]; Celia Machado Ronconi [1]; José Walkimar de Mesquita Carneiro [1]

[1] Universidade Federal Fluminense; [2] Universidade Federal Fluminense

CO2 capture in mixtures of glycerol and nitrogenous bases. We employed theoretical and experimental studies of chemical absorption of CO2 by the glycerol-base system to form glycerol carbonate.

Catecholase-mimetic activity of mononuclear complexes of copper(II)

https://proceedings.science/p/119826

Bruna Luiza Auras [1]

[1] Departamento de Química / Centro de Ciências Físicas e Matemáticas / Universidade Federal de Santa Catarina

Cerium phosphate covered with polyvinylpyrrolidone as UV filter

https://proceedings.science/p/120239

Marrary das Chagas Silva Chagas Silva [1]

[1] USP

Complexo de rutênio contendo tiadiazol derivado do cinamaldeído: síntese, caracterização e avaliação de atividade contra câncer.

https://proceedings.science/p/120578

Maria Isabella Zachi Soares [1]; José Clayston Melo Pereira [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Antitumor activity of ruthenium complex; Development of coordination compound containing organic drug; Potential anticancer activity of thiadiazole.

Complexos polipiridínicos de Ru(II): um estudo teórico e espectroscópico

https://proceedings.science/p/120680

Ana Carolina Cellis do Nascimento [1]; Fabio da Silva Miranda [1]
[1] Instituto de Química / Universidade Federal Fluminense

This work compares the photophysical properties of a family of Ru(II) polypirydyl complexes using XANES, EXAFS, UV-visible spectroscopy, and DFT calculations.

Compostos binucleares de CuII e CoII contendo um ligante quiral: síntese, caracterização espectroscópica, estruturas cristalinas e cálculos teóricos

https://proceedings.science/p/119710

Esther Saraiva Areas [1]; Brunno Freitas [1]; Henrique de Castro Silva Junior [1]; Guilherme Pereira Guedes [1]
[1] Universidade Federal Fluminense

Binuclear complexes containing a chiral 1,3-oxazolidine ligand. DFT calculations predict ferromagnetic interactions between metal cations.

Copper(II) complex containing bis(pyrazole-selenium) ligands: synthesis, X-ray crystallography and antioxidant studies

https://proceedings.science/p/120438

Adriana Castro Pinheiro [1]; Ianka Jacondino Nunes [1]; Daniela Hartwig [1]; Roberta Cargnelutti [2]; Thalita Aquino [1]; Raquel Jacob [1]; Lucielli Savegnago [1]; Angela Maria Casaril [1]
[1] Universidade Federal de Pelotas; [2] Universidade Federal de Santa Maria

Synthesis of Cu(II) complex with bis(pyrazole-selenium) ligand. Molecular structure of complex 2a were confirmed by crystallographic study. Antioxidant activity was determined trough in vitro assays.

Desenho e caracterização de um novo polímero de coordenação heterometálico contendo o ligante bpca

https://proceedings.science/p/120622

Rafaela Maria Ribeiro da Silva [1]; Iara Maria Landre Rosa [1]; Willian Xerxes Coelho Oliveira [2]; Maria Vanda Marinho [1]
[1] Universidade Federal de Alfenas; [2] Universidade Federal de Minas Gerais
• Hydrolysis of the 2,4,6-tris(2-pyridyl)-1,3,5-triazine (tpyt); • Ligands bis(2-pyridylcarbonyl)imide (Hbpca) and carboxylics acids; • Formation of a new 1-D heterometallic coordination polymer.

Desenvolvimento do complexo Cu(bipy)(INH)NO2]Cl com atividade antiparasitária contra os patógenos da leishmaniose e doença de Chagas

https://proceedings.science/p/120562

Dayana Penha [1]; Wendy Medeiros [2]; Johny Oliveira [2]; Ana Brito [2]; Daniel Pontes [2]; Marcelo Silva [2]; Francisco Ordelei Nascimento da Silva [1]
[1] Instituto de Química / Universidade Federal do Rio Grande do Norte; [2] Universidade Federal do Rio Grande do Norte

In this work, the synthesis and characterization of a copper complex with antimonial action against the parasites of leishmaniasis and Chagas disease is presented.

Development of Fricke Gel Chemical Dosimeter with Eriochromo Cyanine R sensitivity to gamma photons and X-rays with high dose of saturation

https://proceedings.science/p/120694

Wandson dos Santos de Almeida [1]
[1] Universidade Federal de Sergipe

The eriochrome cyanine R (RCT) showed excellent properties as a binder in the Fricke gel dosimeter. Increasing the absorbed dose increases the concentration of the Fe3+-ECR complex.

Electrochemical and spectroscopic evaluation of the formation of the Co-Malathion complex

https://proceedings.science/p/120175

Ana Layla Carvalho de Lima [1]; Eliana Maíra Valle [1]
[1] Universidade Federal de São Paulo

In this study, the interaction between the pesticide Malathion and the metal ion cobalt was evaluated by spectroscopic and electrochemical techniques, and both indicated the formation of a complex.

Emission spectroscopy as a probe in the catalysis by EuMOF.

https://proceedings.science/p/120128

Cristiane Kelly de Oliveira [1]; Severino Alves Junior [2]; Ricardo Luiz Longo [2]; Ivani Malvestiti [2]
[1] Universidade Federal de Pernambuco; [2] Universidade Federal de Pernambuco - UFPE

Luminescence spectroscopy is an important probe in assessing the role of the europium ion as catalyst in carbonyl addition reactions.

Estruturas cristalina de complexos de paládio(II) com Bases de Schiff derivadas do salicilaldeído e N,N-dialquil-p-fenilenodiaminas

https://proceedings.science/p/119770

Wladimir Pereira Duarte Badaró [1]; Luís Eduardo Sarto [2]; Eduardo Tonon de Almeida [1]
[1] Universidade Federal de Alfenas; [2] Instituto Federal do Sul de Minas

Há algumas décadas, muitos complexos de metais de transição são investigados devido a suas propriedades antineoplásica e antiparasítica1. Porém, muitos destes medicamentos, como, por exemplo, os derivados da platina, causam efeitos colaterais severos2. Por isso, novos fármacos menos agressivos e mais eficientes é o foco de novos estudos, sendo alguns deles baseados em mudanças estruturais e intercâmbio do metal3. O paládio vem ganhando destaque nessa área, principalmente pela semelhança química estrutural entre o íon Pd (II) e o Pt (II). Embora ambos compartilhem uma configuração d8, a reatividade é bem diferente, sendo os complexos de paládio mais lábeis que os da platina, com uma razão de intercâmbio dos ligantes cerca de 105 vezes maior4. Para minimizar essa labilidade, ligantes quelantes, como as bases de Schiff, têm sido explorados para obter complexos de maior estabilidade cinética. Nesse trabalho foram obtidos novos complexos quelatos de paládio(II) contendo bases de Schiff derivadas de salicilaldeído e N,N-dialquil-p-fenilenodiaminas, reagindo em proporções estequiométricas em meio metanóico. Os ligantes e os complexos foram caracterizados por técnicas espectroscópicas de IV, RMN ^{1}H e $^{13}C\{1H\}$, análises térmicas de TG-DTA, análise elementar e difração de raios X de monocristais dos complexos. Os principais resultados estão na tabela abaixo. A análise espectroscópica mostrou alterações dos sinais referentes à hidroxila e à imina, indicando que o paládio foi coordenado aos ligantes pelos átomos de oxigênio e nitrogênio, formando um anel N, O-quelato. A análise das curvas TG mostra a decomposição dos compostos e a massa residual dos complexos, sendo esta última importante

para a determinação do teor de paládio nos compostos de coordenação sintetizados. As estruturas cristalográficas confirmam as estruturas e os modos de coordenação propostas.

Estudo térmico e DFT de complexos de Pd(II): trans-[PdCl2(HL)(PPh3)] (HL = pirazol (Pz); 4-nitropirazol (NO2Pz); 4-iodopirazol (IPz) e PPh3 = trifenilfosfina)

https://proceedings.science/p/119628

Alessandra Stevanato [1]; Leonardo B. Ribeiro [2]; Adelino Vieira de Godoy Netto [2]; Antonio Eduardo Mauro [2]; Oswaldo Treu-Filho [2]; Cristiana da Silva [3]

[1] Universidade Tecnológica Federal do Paraná - campus Londrina; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [3] Universidade Federal da Grande Dourados

Theoretical calculations (DFT) were performed using the Gaussian program, where the optimized structures the homo and lumo orbitals of the complexes [PdCl2(L)(PPh3)], L- Pz (1), NO2Pz (2) and IPz (3).

Evaluation of the biological potential of novel polypyridinic ruthenium(II) complexes

https://proceedings.science/p/120567

Florêncio Gouveia Júnior [1]; Allandeiverson Santos de Sousa [1]; Barbosa da Silva Renally [2]; Lisa Ridnour [3]; David Wink [3]; Luiz Nascimento Neto [2]; Edson Teixeira [2]; Eduardo Sousa [1]; Luiz Gonzaga de França Lopes [1]

[1] Laboratório de Bioinorgânica / Departamento de Química Orgânica e Inorgânica / Universidade Federal do Ceará; [2] Laboratório Integrado de Biomoléculas / Departamento de Patologia e Medicina Legal / Universidade Federal do Ceará; [3] Cancer and Inflammation Program / National Cancer Institute / National Institutes of Health

New ruthenium-based complexes were synthetized; Compounds were studied through XANES and EXAFS techniques; Complexes show improved cytotoxicity against tumor cells when irradiated with blue light.

Flow synthesis of polynitrogenated ligands and Cobalt(III) complexes of the type [Co(L)(NO2)2] +.

https://proceedings.science/p/119416

Caio Massoto Pacheco [1]; Mauricio Lanznaster [1]

[1] Universidade Federal Fluminense

A flow reactor system was used for preparation of polynitrogenated ligands and their cobalt(III) complexes, in larger scale, greater reproducibility and higher yields than conventional batch reactions

Gamma-Fe2O3 as a photocatalyst in the decomposition of methylene blue: Effect of tartaric acid

https://proceedings.science/p/120476

Francisco Garrido [1]; Henrique Cesar Abreu do Nascimento Telles Rodrigues [1]; Marta Eloisa Medeiros [1]

[1] Universidade Federal do Rio de Janeiro

Magnetic photocatalysts were prepared. The addition of tartaric acid increased the photo Fenton degradation of methylene blue by this photocatalyst. These materials can be easily recovered and reused

Gas sensor based on Mn3O4/ZnO heterostructure for butanone detection

https://proceedings.science/p/120505

Taís Nascimento Teixeira Oliveira [1]; Cecilia de Almeida Zito [1]; Tarcísio Micheli Perfecto [1]; Diogo Paschoalini Volanti [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

The microwave-assisted hydrothermal method, in conjunction with the ultrasonic spray used in the synthesis. Sensor-based on M3O4/ZnO heterostructure with improved detection of butanone.

Hybrid hydrogels based on polyethylene glycol bioconjugated with silylated-amyloidogenic peptides

https://proceedings.science/p/119943

Wendel Andrade Alves [1]; Carla C. Decandio [1]; Sandra Valeria Vassiliades [1]; Barbara Bianca Gerbelli [1]; Andrea M. Aguilar [2]
[1] Universidade Federal do ABC; [2] Universidade Federal de São Paulo

A simple sol-gel functionalization method through PEGylation in the presence of one amyloid-like peptide is presented.

Influência do solvente na síntese de novos polímeros de coordenação baseados no ácido 2,5-piperazinediona-1,4-diacético e íons Tb3+

https://proceedings.science/p/120411

Luana Reine Pinheiro Lima Cunha [1]; Fausthon Fred da Silva [1]
[1] Universidade Federal da Paraíba

The influence of the solvent in the obtention of coordination polymers was studied. Four new Tb3+ based structures were obtained using 2,5-piperazinadione-1,4-diacetic acid and oxalic acid as ligands.

INVESTIGAÇÃO DE COMPLEXOS DO TIPO COBALTO(III)-β-DICETONAS COMO PROTÓTIPOS DE METALOFÁRMACOS ATIVADOS POR HIPÓXIA

https://proceedings.science/p/119712

Carolina Alonso Pereira [1]; Marcos Vinicius Palmeira Mello [2]; Myrthes Carvalho [3]; Mauricio Lanznaster [3]
[1] Instituto de Química/ Universidade Federal Fluminense; [2] Universidade Federal Fluminense / Instituto de Química; [3] Universidade Federal Fluminense

β-diketones can be used as a model of antitumor drugs in cobalt (III) complexes. Therefore, three complexes with β-diketones, functionalized with anilines, were synthesized and characterized.

Investigation of DNA interacting properties and in silico studies of copper(II) and palladium(II) chloride complexes

https://proceedings.science/p/119711

Marcos Vinicius Palmeira Mello [1]; Ana B. Caballero [2]; Aida Lopez Espinar [2]; Guilherme Pereira Guedes [3]; Amparo Caubet [2]; Alessandra Mendonça Teles de Souza [4]; Mauricio Lanznaster [3]; Patrick Gamez [2]
[1] Universidade Federal Fluminense / Instituto de Química; [2] Universitat de Barcelona; [3] Universidade Federal Fluminense; [4] Universidade Federal do Rio de Janeiro

Two Cu2+ and Pd2+ complexes were evaluated as DNA-binder. Different DNA-interacting modes were proposed for these compounds. High cleavage potential was observed. Molecular docking was also performed.

Isoreticular approach in the synthesis of a new 3D Mn2+ coordination polymer based of trimesic acid: structural and topological studies

https://proceedings.science/p/120475

Gabriel Barbosa Souza [1]; Charlane Cimini Corrêa [1]; Leonã da Silva Flores [1]
[1] Universidade Federal de Juiz de Fora

This work presents one coordination polymer (CP), named as 1 with an unusual topology, and obtained from the attempt of isoreticular synthesis SBU modification using a template.

Material Híbrido para Detecção de Aminas Aromáticas Heterocíclicas

https://proceedings.science/p/120572

Sueslley Rodrigues [1]; Leandro Araújo [2]; Maria Karolina da Silva Oliveira [2]; Monilson Pinheiro [3]; Luiz Henrique da Costa Souza [4]; Elisane Longhinotti [3]; Izaura Cirino Nogueira Diogenes [1]; Maria Aparecida [3]
[1] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica; [2] Universidade Federal do Ceará; [3] UNIVERSIDADE FEDERAL DO CEARÁ; [4] UFC (Universidade Federal do Ceará)

A hybrid material composed of [Fe(CN)5(NH3)]3- adsorbed on chitosan was used as colorimetric sensor for detection of quinoxaline, a carcinogen HAA type compound produced during meat processing.

Mechanistic studies of isonicotinate formation from isoniazid-cyanidoferrate complexes in salt-rich solutions

https://proceedings.science/p/120213

Marcio Cristiano Monteiro [1]; Bruno Szpoganicz [1]; Roselene Kroth [1]; Thiago Caon [1]
[1] UFSC

Although the isoniazid (INH) has been the most widely used antituberculostatic prodrug due to its high efficacy, problems of microbial resistance are frequently observed[1]. In this context, its complexation with transition metal (Fe) could be used in order to overcome this drug limitation. In fact, the use of the pentacyanidoferrate(II)-INH complex (PCF-INH) has demonstrated to be effective in inhibiting resistant strains of Mycobacterium tuberculosis; however, the mechanism which involves the transformation of INH into isonicotinoyl radical is not completely understood yet[2] . Once the PCF-INH complex needs to be transported in different organic systems until it achieves lung, stability studies in different salt-rich aqueous media were performed (phosphate buffered saline-PBS and PBS/trichloroacetic acid-TAA). The TAA was used to simulate more acid regions (e.g. stomach). In addition to assays with the PCFINH, a Prussian blue derivate containing INH (PB-INH) was also considered. Results showed INH oxidation and isonicotinate (ISN) formation in both solutions (Fig. 1a-b). For the PCF-INH, INH can be changed for H2O in coordination sphere. This complex can be oxidized[3] and then reacting with PCF-INH and free INH, resulting in PCFISN and ISN formation, respectively. PCF-ISN also can changes ISN ligand for H2O, releasing ISN to solution (Fig. 1c). In PB-INH complex, phosphate ions from PBS solutions reacts with Fe(III), breaking PB-INH structure, forming PCF-INH. Fe(III), in excess, can easily oxide free INH and PCF-INH, resulting in ISN and PCF-ISN formation, even in TAA presence (Fig. 1d). Taking together, these results demonstrate that salt-rich buffering medium (neutral and acid) can provide isonicotinoyl radical (and then ISN) by INH oxidation.

Mechanochemical synthesis of europium complexes

https://proceedings.science/p/120138

Jéssika Cavalcanti de Lima [1]; Sarah P. da Silva [1]; Ricardo L. Longo [1]; Ivani Malvestiti [1]
[1] Universidade Federal de Pernambuco

New europium complexes were synthesized with N-acetylbenzamide and 2-benzyl-1,3-diphenylpropane-1,3-dione as ligands by mechanochemical method, as new green synthetic route.

Mesoporous silica HMS as support of Mn-porphyrins for oxyfunctionalization of cyclohexane and n-heptane

https://proceedings.science/p/119420

Isaque Feitosa [1]; Julio Santos Reboucas [2]; Shirley Nakagaki [3]; Victor Pinto [2]
[1] Departamento de Química / Centro de Ciências Exatas e da Natureza / Universidade Federal da Paraíba; [2] Universidade Federal da Paraíba; [3] Departamento de Química / Setor de Ciências Exatas / Universidade Federal do Paraná

Mn-porphyrins were anchored on silica HMS via electrostatic or covalent bond. Catalysts oxidized cyclohexane and n-heptane. MnP loadings were kept at low level (0.3% w / w) were selective for alcohol.

Modificação de superfície de ouro com nanopartículas magnéticas acopladas a Concanavalin A para detecção de bactérias

https://proceedings.science/p/120568

Leandro Araújo [1]; Maria Karolina da Silva Oliveira [1]; Maria Aparecida Santiago [1]; Sueslley Rodrigues [2]; Vitória Soares [1]; Izaura Cirino Nogueira Diogenes [2]
[1] Universidade Federal do Ceará; [2] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica

Nanocomposite of CoFe2O4 magnetic nanoparticles functionalized with amine and lectin was successfully anchored on gold electrodes envisioning E. Coli detection.

Monolayer of 1,4-benzenedithiol on gold: A platform for gold nanoparticles immobilization

https://proceedings.science/p/120546

Vitória Dibo [1]; Clara Vasconcelos [1]; Leandro Araújo [2]; Lucas Bezerra [1]; Izaura Cirino Nogueira Diogenes [3]
[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Universidade Federal do Ceará; [3] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica

Gold polycrystalline surfaces were spontaneously modified with sulfur molecules to construct platforms of electrochemical biosensors including the incorporation of gold nanoparticles.

NON-COVALENT INTERACTIONS STUDY BETWEEN SI-PPC AND BIOMOLECULES THROUGH A THEORETICAL MOLECULAR DYNAMICS APPROACH

https://proceedings.science/p/120518

Frederico Henrique do Carmo Ferreira [1]; NATHALIA MAGALHAES ROSA [1]; Luiz Antônio S. Costa [1]
[1] Universidade Federal de Juiz de Fora

To evaluate chemistry properties of platinum complexes that would lead to an active antitumor activity due to non-covalent interactions with biomolecules targets that play important roles in cells.

Novo Complexo Binuclear de Cobre (I) Baseado em Ligantes Bifosfina/Pirazolina com Promissora Aplicação Antitumoral

https://proceedings.science/p/120564

Gleison Antônio Casagrande [1]; Cristiane Freitas de Almeida Teixeira [1]; Katia Tenório [1]; Lucas Pizzuti [2]; Vinicius Oliveira [1]; Victor Marcelo Deflon [3]; Izamara Casadia [2]
[1] Universidade Federal de Mato Grosso do Sul; [2] Universidade Federal da Grande Dourados; [3] USP - São Carlos

The copper (I) binuclear complex was synthesized and structurally characterized by X-ray diffraction and In vitro cytotoxicity assays showed that the complex presented promising antitumor activity.

On conformational isomerism of a Ru(II) complex and potential anticancer activities to its derivatives.

https://proceedings.science/p/119470

Leticia Pires De Oliveira [1]; Gabriel Henrique Ribeiro [1]; Carlos André Ferreira Moraes [1]; João Honorato [1]; Eduardo Ribeiro de Azevedo [2]; Alzir Azevedo Batista [3]
[1] Universidade Federal de São Carlos; [2] Universidade de São Paulo; [3] Universidade Federal de São Carlos/Universidade Federal de Goiás

Ruthenium complexes have been excelled for demonstrating potential activity against cancer and against infectious diseases.1 Thus, one approach in the field of cancer is related to the target of the agent on study. In this case, should be

good to know how the drug, or the potential drug, interacts with the target, by which mecanism, and to know if the compound acts inside, or outside the cell, for instance. Trying to answer some of these questions, in this work new ruthenium complexes with fluorescence properties, were synthesized, and for this a pyrene(py) derivative, a quimiosensor specie, was used as ligand.2 The new ruthenium complexes have in their coordination sphere, basically, the 1,4-bis(diphenylphosphino)butane, 2-(1-pyrenil)1H-imidazo[4,5-f][1,10]-phenantroline (pyphen), using the chloride complex as precursor (see Fig. 1). To complete the coordination sphere of the metal, mercapto ligands were used (Complex A2, Fig. 2). It is interesting to mention that the 31P{1H} NMR spectrum of the precursor showed a complex pattern, different of the expected for a AX system, suggesting that more than one specie was in solution, according Fig. 3. Also, the spectra of the complex are a little different, depending of the solvent used in the experiment. The hypothesis of the presence of more than one compound in solution was discarded by cyclic voltammetry experiments, where only one oxidation process, Ru(II)→Ru(III), was observed, which was supported by mass spectra data. In order to evaluated the presence of possible isomers of the precursor, in solution, NMR spectra, in solid state, were undertaken, and the results suggest the presence of conformational isomers, which was confirmed by 31P{1H} experiments, where at least five signals were observed. Additionally, worth it to mention that the reaction of the precursor with the mercapto ligand (complex A2), only one complex was obtained, again, suggesting that in the precursor solution only one specie was present. Worth it to mention that, the obtained complexes are fluorescent, and can be used as probe to study the mechanism of their interaction with the cancer cells. 1HONORATO, J. et al. Inorg. Chem. Front. v. 6, p. 376-390, 2019. 2RANIK,B.K.; JOHN, S.A. J. Hazard. Mater. v. 343, p. 98-106, 2018.

Otimização das condições sintéticas para a obtenção de estruturas metalorgânicas (MOFs) em temperatura ambiente

https://proceedings.science/p/120596

Larissa Daniela Dias Rafael [1]; Iara Maria Landre Rosa [1]; Maria Vanda Marinho [1]
[1] Universidade Federal de Alfenas

Metal-organic frameworks, for industrial application, can be obtained at room temperature and reduced reaction time. Synthetic conditions affect directly the obtaining of metal-organic networks.

PdII and AgI complexes with curcumin as anticancer and antibacterial candidates

https://proceedings.science/p/119495

Jocely de Lucena Dutra [1]; João Honorato [1]; Alzir Azevedo Batista [1]
[1] Universidade Federal de São Carlos

Synthesis, characterization and evaluation of anticancer and antibacterial activity of palladium and silver complexes with curcumin and triphenylphosphine ligands.

PdII Complexes containing diimine ligands: synthesis, characterization and catalytic activity in Heck type reactions.

https://proceedings.science/p/120170

Raíza Fonseca Xavier Lima [1]
[1] Universidade Federal do Triângulo Mineiro

Photochemical generation of singlet oxygen by a ruthenium complex containing an anthracene derivative

https://proceedings.science/p/120570

Monilson Pinheiro [1]; Lucas Bezerra [1]; Bruna Talia dos Santos Carvalho [2]; Lucas Rodrigues Viana [3]; Idalina M. M. Carvalho [1]; Izaura Cirino Nogueira Diogenes [2]
[1] UNIVERSIDADE FEDERAL DO CEARÁ; [2] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica; [3] Universidade Federal do Ceará

Ruthenium complex containing a highly aromatic anthracene derivative was used to photochemically produce singlet oxygen giving quantum yields as high as 1.0

Photoluminescent study and cytotoxicity assay of red iridium-emitting complexes

https://proceedings.science/p/119936

Felipe da Silva Manrique Canisares [1]; Alessandra M. G. Mutti [2]; Dalita G. S. M. Cavalcante [2]; Aldo E. Job [2]; Ana Maria Pires [3]; Sergio A Marques de Lima [4]

[1] Instituto de Química - UNESP; [2] FCT - UNESP; [3] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [4] Universidade Estadual Paulista-Unesp

Cyclometallating Iridium(III) complexes have showing great attractiveness to biological assays due to some photoluminescent properties such as large Stokes shift, long luminescent lifetimes, great photostability and good permeability to cell membranes[i]. As luminescent biomarkers, these complexes may represent an alternative to replace organic dyes which exhibit small Stokes shifts, low photostability and in most cases the excitation wavelength is high enough to cause damage in living cells. Considering that biological tissues are not transparent to blue and green, red and infrared emitters are better options to record biological images.[ii] Therefore, in this work, we synthesized two red emitters Ir(III) complexes: (i) [Ir(ppz)2(bpdc)] and (ii) [Ir(ppz)2(bqdc)], using carboxylic acid ligands as ancillary ligands. To obtain the complexes the first step was the cyclometallation of Ir(III) as dimmer, [(ppz)2(μ-Cl)2(ppz)2], performed through the Nonoyama route[iii]. In the second step the ancillary ligands (bpdc or bqdc) and K2CO3 in excess were dissolved in water and mixed in the dimmer solution dissolved in dichloromethane; then, methanol was added resulting in a monophasic system, and both complexes were precipitated by addition of hexane. The complexes were purified in silica gel column and characterized by FTIR, UV-Vis, MALDI-TOF and 1H-NMR. Photoluminescence properties were recorded in ethanol (at 77 K and 300 K) and in PBS (300 K) solution (phosphate buffered saline). In PBS solution both complexes, [Ir(ppz)2(bpdc)] and [Ir(ppz)2(bqdc)], show emission in the red spectral region characterized by a broadband centered at 625 nm and 659 nm, and CIE color coordinates of (0.612;0.336) and (0.635;0.252); the measured quantum yield were 2.1% and 15.9%, respectively, and the second one displays one of the highest quantum yield recorded in aerated solution at room temperature reported in literature[iv]. To demonstrate their biological application, citotoxicity tests were investigated in CHO-k1 cells line of rat ovarian fibroblast in different concentrations; the lowest concentration in which the complexes are considered nontoxic are 100 μg/mL (87% of cell viability) for [Ir(ppz)2(bpdc)], and 25 μg/mL (100% cell viability) for [Ir(ppz)2(bqdc)], evidencing their potential in biological assays as luminescent biomarker for cell imaging. [i] Q. Zhao, M. Yu, L. Shi, et. Al. Organometallics 2010, 29, 1085–1091 [ii] A. M., Mancini, M. C., Nie, S. Nature Nanotechnology, 2009, 4(11), 710–711 [iii] M. Nonoyama, Bull. Chem. 156 Soc. Jpn., 1974, 47, 767–768 [iv] W. Jiang, Y. Gao, Y. Sun, et. Al., Inorg. Chem. 2010, 49, 3252–3260

Photophysical properties and ligand effective polarizabilities in β-diketonate lanthanide complexes with phenanthroline.

https://proceedings.science/p/120077

Paulo Roberto da Silva Santos [1]; Dariston Kleber Sousa Pereira [2]; Ercules Epaminondas de Sousa Teotonio [2]; Israel Ferreira da Costa [2]; Iran Ferreira da Silva [2]; Wagner Mendonça Faustino [2]; Renaldo Moura Jr [2]; Albano Neto Carneiro Neto [3]; Hermi Felinto de Brito [4]; Maria Helena Araujo [5]; Renata Diniz [5]; Oscar Manoel Loureiro Malta [6]

[1] Universidade Federal da Paraíba ; [2] Universidade Federal da Paraíba; [3] Universidade de Aveiro; [4] Universidade de São Paulo; [5] Universidade Federal de Minas Gerais; [6] Universidade Federal de Pernambuco

This work reports on the synthesis, characterization, and photophysical properties of the lanthanide compounds of general formula [Ln(β-dik)(NO3)2(phen)2], where β-dik = acetylacetone (acac), hexafluoroacetone (hfac), tenoyltrifluoroacetone (tta) and bezoylacetone (bzac), phen = 1-10-phenanthroline, and Ln = Eu3+ and Gd3+. These complexes were prepared by direct reaction among methanolic solutions of the Ln(NO3)3·6(H2O), β-dik and phen ligands in the ratios Ln:β-dik:phen of 1:1:2.[1] All complexes were characterized by complexometric titration with EDTA, CHN microanalysis, absorption spectroscopy in the infrared region (IR), thermogravimetric analysis, diffuse reflectance in the UV-Vis region and luminescence spectroscopies. The properties of the [Ln(β-dik)(NO3)2(phen)2] complexes were compared with those ones for the [Ln(β-dik)3(phen)] complexes. The [Eu(acac)(NO3)2(phen)2]·H2O compound had its molecular structure elucidated by the single-crystal x-ray technique, presenting the following cell parameters: Space group: P2/n; a(Å) = 11,1982; b(Å) = 9,7154; c(Å) = 13,3217; α(o)= 90,0; β(o)=101,569; (o)=90,0; V(Å3)=1419,94; Z=2. Diffuse reflectance spectra of the [Ln(β-dik)(NO3)2(phen)2] complexes showed an additional broad band, which may be assigned to a low energy LMCT state. The emission and excitation luminescence spectra, recorded at 300 and 77 K, were used to calculate the experimental intensities parameters and intrinsic quantum

efficiency of Eu3+ complexes. Concerning the theoretical part of the work, geometries of the complexes were optimized at Sparkle/AM1 level and the localized molecular orbitals (LMO's) were achieved using the Pipek-Mezey procedure. The contribution from each LMO to the total molecular polarizability ( ) was calculated using B3LYP/aug-cc-pVDZ method with the GAMESS program. The effective ligand polarizabilities (') values were calculated by adding up the polarizabilities from each LMO's in specific regions near the atoms directly coordinated to the lanthanide ion. The effective polarizabilities data obtained for the isolated ligands showed that the α' values for the nitrate ligands are lower values than those for the other ligands, probably because of their small size and high hardness. It was also observed that the substituent groups in the β-diketonate ligands play an important role on the α' values. Interestingly, the asymmetric β-diketonates tta and bzac presented different α' values for each oxygen donor atoms, whereas both oxygen donor atoms in the symmetric β-diketonates acac and hfac ligands exhibited similar α' values. The values of polarizabilities in specific regions near the atoms directly coordinated to the lanthanide ion, together with charge factors (g) of donor atoms, were used for calculate theoretical intensity parameters, which were compared with those determined experimentally from the luminescence spectral data.

Polímeros de Coordenação Aniônicos Baseados em Ácido Piromelítico e Poliaminas

https://proceedings.science/p/120554

José Rafael Costa Ferreira [1]; Charlane Cimini Corrêa [1]; Filipi Joaquim Teixeira [1]; Leonã Silva Flores [1]
[1] Universidade Federal de Juiz de Fora

Synthesis and characterization of coordination polymers; Studies of the effects of alkyl-ammonium cations on CP design; Potential applications explain the growing interest as functional materials.

Porphyrins immobilized in TiO2: photocatalysts in the antibiotic levofloxacin degradation

https://proceedings.science/p/119487

Aline Capelão Marciano [1]; Ana Luísa Almeida Lage [1]; Ana Flávia da Silva Reis [1]; Mirra Angelina Neres da Silva [1]; Dayse Carvalho Da Silva Martins [1]
[1] Universidade Federal de Minas Gerais

Due to technological advances and population growth in recent decades, the amount of antibiotics detected in effluents has been increased. Their effects can already be seen, such as the appearance of super bacteria, which contributes to antibiotic resistance, and genetic mutations of aquatic beings.1 Therefore, the non-aggressive elimination of such drugs becomes extremely important. The degradation of the antibiotic levofloxacin (LEV, Fig. 1a) was evaluated in the presence of Oxone®, by using the porphyrins H2T4CPP (P1) and H2T4SPP (P2) as photocatalysts (independently), in an homogeneous system or in its immobilized form on inorganic support TiO2 (Fig. 1b). The materials containing TiO2 and the catalyst were obtained by immobilizing the porphyrins in the support, independently, using methanol as solvent. The materials are going to be characterized by X-Ray Diffraction and Scanning Electronic Microscopy. In general, the presence of the oxidant Oxone® contributed to greater degradation of the LEV (Fig. 2), with an increase of 42 to 163% in relation to the respective systems in absence of oxidant. The heterogeneous systems resulted in the greatest degree of LEV degradation. The immobilization of porphyrins led to a relative increase in LEV degradation of 45 to 204% in relation to homogeneous systems in the presence of the oxidant, for P1 and P2, respectively. The advantage of these systems is the recovery and reuse of the catalyst, which is under development at the moment. Furthermore, in homogeneous catalysis, a deactivation of the catalyst may occur, which can be caused by bimolecular interactions in solution, which could promote the formation of highly stable and inactive μ-oxo dimer species or the oxidative destruction of the porphyrinic macrocycle1. These factors could justify the lower degradation of the LEV in homogeneous systems. Therefore, the association between porphyrins and TiO2 is promising for the development of systems for the degradation of environmental contaminants. The next steps of this study are related to the study of other sources of irradiation and to investigate the use of other porphyrin catalysts, which can increase the degradation of antibiotics and other contaminants in heterogeneous systems. 1Environmental Pollution 225 (2017) 304-315; 2Chemical Reviews 92 (1992) 1411-1456. Acknowledgments UFMG, Capes, CNPq, FINEP, and FAPEMIG

Potential catalyst for water splitting: theoretical and experimental study with Nickel complexes.

https://proceedings.science/p/120458

Gabriel Aguiar de Souza [1]; Naiara Adolpho de Lima [1]; Naheed Bibi [2]; Andre Formiga [1]
[1] Universidade Estadual de Campinas; [2] Shaheed Benazir Bhutto Women University

In this work, we studied the potential catalytic activity of nickel complexes with ligands bearing three imidazole units. TD-DFT calculations support the experimental results.

Preparação e estudo por docking e fotofísica de um novo metalointercalante contendo Ru(II) complexado ao ligante dppzBTDZ

https://proceedings.science/p/119885

Mariana de Oliveira Tonelli Nogueira [1]; Pedro Henrique Luciano da Silva [2]; Thamires da S. Luiz [2]; Joyce Sobreiro Francisco Diz de Almeida [1]; Tanos Celmar Costa França [1]; Fabio da Silva Miranda [2]
[1] Instituto Militar de Engenharia; [2] Universidade Federal Fluminense

Synthesis, docking, UV-Vis and emission DNA studies of new metallo-intercalator of Ruthenium(II) complex with planar ligand derivate from 1,10-phenanthroline as a promising DNA probe.

Preparation of metalloporphyrin-based layered/magnetic solids to catalyze one-pot sequential reaction for cyclic carbonate generation

https://proceedings.science/p/120528

Everton Henrique dos Santos [1]; Fernando Wypych [1]; Shirley Nakagaki [1]
[1] Departamento de Química / Setor de Exatas / Centro Politécnico / Universidade Federal do Paraná

In this work it is investigated the preparation of catalyst solids for epoxidation reaction and cyclic carbonate formation based on the immobilization of iron(III)porphyrin in inorganic solid supports

Preparation of nanostructured systems by self-assembly of nanoparticles

https://proceedings.science/p/119497

Mariana Enacles de Abreu [1]; Mario Roberto Meneghetti [1]; Monyque da Alves [1]
[1] Universidade Federal de Alagoas

Gold nanoparticles (AuNPs) are considered materials of great interest due to their singular properties that are strongly dependent of their size and shape. However, the environment around of these particles also produces effects that tune or change completely the properties of the nanostructured systems, e.g. solvents, surfactants, particle concentration, etc. In this sense, this work aims to develop methodologies to attain nanostructured materials via tailor-made self-assembling processes, using AuNPs with different morphologies as building blocks. The spherical AuNPs (AuNSs) were synthesized by the Turkevich method (13 nm in diameter) and the rod-like AuNPs (AuNRs) were obtained by seed mediated method, according to the protocol developed by the El-Sayed group (45 x 15 nm), and their colloids showed characteristic UV-vis absorption spectra. To induce a specific process of self-assembly of AuNSs and AuNRs, we modified the surface of each AuNPs type with specific molecules with suitable functional groups - Cysteamine (CYS) contain amine and thiol groups and Mercaptoacetic acid (AMA) contain carboxylic acid and thiol group. After surface modification, the two sets of AuNP colloids were mixed, i.e. AuNS/CYS and AuNR/AMA together with EDC and NHS to allow C-N bond formation. We noted that after mixing, the Uv-vis absorption spectra of the mixture radically changed. This was not just a superposition of the two previous spectra before mixing. This characteristic suggest that particle interactions are in process. Nevertheless, until now, under dry conditions, the expected self-assembled arrange was not observed (on TEM grids). Further studies on sample preparation are in progress.

PSI-MS Combined with DFT Calculations to unveil the Zirconium Speciation in Acid Aqueous Solution

https://proceedings.science/p/120483

Alexandre Bertoli [1]; Ana Gabriella Carvalho Miguita [1]; Rodinei Augusti [1]; Helio Anderson Duarte [1]
[1] Universidade Federal de Minas Gerais

Paper spray ionization to detect species of Zr(IV). DFT confirms the nature and stability of Zr(IV) in the presence of NO3- and F- ions. The fluoroanions of Zr(IV) are resistant to hydrolysis.

Red-light-emitting Langmuir–Schaefer films based on highly-hydrophobic Eu3+ tetrakis-β-diketonate complexes containing amphiphilic counter-ions

https://proceedings.science/p/119963

Airton Germano Bispo Junior [1]; Camila M. B. Leite Silva [2]; Sergio A. M. Lima [3]; Lucas V. L. Citolino [2]; Clarissa A. Olivati [2]; Ana Maria Pires [4]
[1] São Paulo State University, Institute of Chemistry, Araraquara, Brazil; [2] UNESP; [3] UNES; [4] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Luminescent thin films containing Eu3+ β-diketonate complexes fabricated by the Langmuir-Schaefer (LS) technique find several applications such as in light-converting molecular devices or in solid-state lighting.[1] However, the main challenge concerning their fabrication lies in the deposition control and homogeneity of the films since the complexes usually display high hydrophobicity.[2] To overcome this issue, in this study, we have investigated the fabrication of LS films based on [Q][Eu(dbm)4] complexes (Hdbm = 1,3-diphenyl-1,3-propanedione, Q1 = C26H56N+, Q2 = C19H42N+, or Q3 = C17H38N+)[3],[4] in order to use amphiphilic counter-ions to organize the luminescent anionic complex on the subtract. To fabricate the LS films, a basin was used with ultrapure water in the liquid subphase at 25 ºC. For the fabrication of each film, a certain amount of the complex in chloroform was spread out on the aqueous subphase. After the solvent evaporation, it got started the movable barrier compression at constant velocity of 10 mm.min-1. Along with the compression process, surface pressure versus mean molecular area (π-A) isotherms were obtained. The complex was transferred to the hydrophilic glass substrate in the horizontal position by using the deposition mode called Z-type, under surface pressure of 20 mN.m-1. For all films, 11 layers were deposited onto the substrates, monitored by UV-VIS absorption spectra. The amphiphilic counter-ions play an important role in the film fabrication by increasing the surface homogeneity and deposition quality as the carbonic chain increases, especially for the [Q1][Eu(dbm)4] film, which showed a root mean square surface roughness of 37.8 nm recorded by atomic force microscopy. All films displayed the characteristic Eu3+ red-light emission under excitation at 367 nm, and the best 5D0 state quantum efficiency of Eu3+ was achieved for the [Q1][Eu(dbm)4] film (27.5 %), confirming that the counter-ion also influences the luminescent properties of the films due to changes in the complex conformation.

Reversible water harvesting by a cobalt(II) 1,2,4-triazole coordination complex

https://proceedings.science/p/119829

Dayenny Louise D'Amato Leite [1]; Catiúcia R. M. O. Matos [1]; Acácio Silva de Souza [2]; Sérgio Pinheiro [3]; Célia Machado Ronconi [4]
[1] Universidade Federal Fluminense, Departamento de Química Inorgânica; [2] Universidade Federal Fluminense, Departamento de Tecnologia Farmacêutica; [3] Universidade Federal Fluminense, Departamento de Química Orgânica; [4] Universidade Federal Fluminense

The cobalt(II) 1,2,4-triazole coordination complex was synthesized and structurally characterized by X-ray diffraction analyses and its reversible water adsorption capacity was evaluated.

Ruthenium (II)/phosphine complexes containing mercapto ligands: synthesis, characterization and citotoxicity against breast cancer cells

https://proceedings.science/p/119466

Analu Rocha Costa [1]; João Honorato [1]; Alzir Azevedo Batista [2]
[1] Universidade Federal de São Carlos; [2] Universidade Federal de São Carlos /

Cancer is a worldwide public health problem, and it is the second leading cause of death in the world. Current drugs on the market have a number of insufficiency, with side effects being the most striking1,2. Therefore, the search for new

drugs that are more effective and that reduce problems related to side effects has been widely explored. In the present work, new ruthenium (II)/phosphine complexes containing mercapto ligands were synthesized and characterized. The compounds, with general formula, [Ru(N-S)(cdppen)(bipy)], were synthesized from the precursor cis- [RuCl2(cdppen)(bipy)] (cdppen = 1,2-bis(diphenylphosphino)ethylene; 2,2'-bipyridine (bipy); N-S = 2-mercapto pyrimidine, 2-mercaptopyridine or 2-mercaptothyazoline ligands), Scheme1. The complexes were characterized by several techniques: molar conductivity, FTIR spectroscopy, cyclic voltammetry, 1H, 13C and 31P{1H} NMR, and monocrystal X-ray diffraction. Conductance measurements in dichloromethane indicated that the complexes are 1: 1 electrolytes (complex 1 = 43.0 ohm-1 cm2 mol-1 and complex 2 = 36.7 ohm-1 cm2 mol-1 at 25 °C), confirming the presence of PF6 - counter ion in the compounds. Based on the 31P{1H} NMR spectra, it is possible to observe the expected doublets, confirming presence of complexes of AX systems. The voltammograms of the complexes, obtained in dichloromethane (1 mmol of PTBA), showed the oxidation potentials of RuII/RuIII, presenting quasi-reversible processes. The complex with the 2-mercaptopyrimidine ligands, is cytotoxic (IC50 = 1.21 ± 0.69 μM) against tumor line MDA-MB-231.The cytotoxicity of the complexes, in cancer and non cancer cells are in progress, and will be showed.

SÍNTESE DE CARBONATOS CÍCLICOS A PARTIR DE CO2 E EPÓXIDOS CATALISADA POR COMPLEXOS METÁLICOS COM LIGANTES BENZOTIAZOIS

https://proceedings.science/p/120537

Álvaro Farias Arruda da Mata [1]; Rafael Pavão das Chagas [1]; Jorge Luiz Sônego Milani [2]
[1] Universidade Federal de Goiás; [2] Universidade Federal de Juiz de Fora

- Facile synthesis of complexes from various metal salts with benzothiazoles ligands.
- Use of benzothiazole complexes as catalysts for the chemical fixation of CO2.

Síntese de carbonatos cíclicos de CO2 e epóxidos catalisados por porfirazinas-MgII

https://proceedings.science/p/120607

Julia Poliana da Silva Caldas Leal [1]; Jorge Milani [1]; Thiago Teixeira Tasso [2]; Laura Rezende [1]; Rafael Pavão das Chagas [3]; Werberson de Almeida Bezerra [3]; Chris Hebert de Jesus Franco [1]
[1] Universidade Federal de Juiz de Fora; [2] Universidade Federal de Minas Gerais; [3] Universidade Federal de Goiás
- High active and selective catalysts; - First report using porphyrazines for chemical fixation of CO2.

Síntese de um novo ligante contendo 1 sítio de coordenação e 2 grupos cromóforos para aplicação em DSSC

https://proceedings.science/p/119953

Caroline Teixeira Guedes [1]; Fabio da Silva Miranda [1]
[1] Universidade Federal Fluminense
Combination of the 1H-Imidazo[4,5-f][1,10]phenanthroline and BODIPY chromophores. Intramolecular charge transfer for application in DSSC. Two chromophores molecule to tune excited states properties.

Síntese e Caracterização de Complexos de Cobre(II) com bases de Schiff derivadas da 1,2-diamino-3,5-dimetilbenzeno e de salicilaldeídos

https://proceedings.science/p/119999

Leona Carolina da Silva Marques [1]; Igor Vinicius de França [1]; Thiago Henrique Döring [1]; Cleber Messias Pires [1]; Edward Ralph Dockal [2]; José Wilmo da Cruz Junior [1]
[1] Universidade Federal de Santa Catarina; [2] Universidade Federal de São Carlos
As Bases de Schiff são iminas resultantes da condensação entre aminas primárias e substâncias carboniladas, cujos complexos possuem variadas aplicações, devido à sua grande variabilidade estrutural. Quatro complexos mononucleares de Cu(II) foram sintetizados, utilizando bases de Schiff tetradentadas derivadas da 1,2-diamino-3,5-dimetilbenzeno e: salicilaldeído, 3-metoxisalicilaldeído, 4- metoxisalicilaldeído e 5-metoxisalicilaldeído (Figura 1)

mediante procedimentos descritos na literatura. Foram caracterizados por medidas de ponto de fusão, testes de solubilidade, medidas de condutividade, espectroscopias no infravermelho e no ultravioleta-visível. Os dados gerais dos complexos estão apresentados na Tabela 1. Os quatro complexos analisados são solúveis em DMF, sendo insolúveis em água. Nas análises de ponto de fusão os complexos se degradaram, ao invés de se fundirem. Nas medidas de condutividade, em DMF, observou-se que todos se mostraram não-eletrólitos. Os espectros eletrônicos apresentaram bandas de alta absortividade, atribuídas às transições $\pi \rightarrow \pi^*$ na região entre 280 nm – 430 nm. Foram observadas bandas d-d para o cobre(II) na região entre 630 nm e 660 nm. Notou-se que as bandas relativas aos estiramentos C=N, C-N e C-O apresentaram-se respectivamente em: (A)1602 cm-1 , 1482 cm-1 e 1318 cm-1 ; (B) 1603 cm-1 , 1461 cm-1 e 1243 cm-1 ; (C) 1607 cm-1 , 1448 cm-1 e 1261 cm-1 ; e (D) 1605 cm-1 , 1489 cm-1 e 1224 cm-1.

Síntese e caracterização de complexos fotoluminescentes de Eu(III), Tb(III) e Gd(III) com ácido 3-tiofenoacético e 4,4'-dimetil-2,2'-bipiridina

https://proceedings.science/p/120499

Eduarda Couto Queiroz [1]; Flávia Cavalieri Machado [1]; Ricardo Oliveira Freire [2]; Monica Dos Santos Ferreira [3]
[1] Universidade Federal de Juiz de Fora; [2] Universidade Federal de Sergipe; [3] Universidade Federal de Sergipe
[Ln2(3-TFA)6(dbp)2] complexes were synthesized. The XRD data showed complexes with dimeric structure. Photoluminescence studies show that Eu(III) complex presents 34% of quantum efficiency.

Síntese e caracterização de complexos mistos de ligantes de tenoiltrifluoroacetonato e difenilfosfinatos com íon Európio(III)

https://proceedings.science/p/120617

Douglas Scarabello [1]; Marco Aurélio Cebim [1]; Vagner Moralles [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"
Formation a new mixed complex of diphenylphosphinate and thenoyltrifluoroacetonate; The mixed of the ligands can increase the europium luminescence; Probable formation of coordination polymeric;

Síntese, caracterização e estudo fotolítico do complexo cis-[Ru(bpy)2(1-meimN)(4-pyCOH)](PF6)2

https://proceedings.science/p/120592

Walysson Pereira [1]; Florêncio Gouveia Júnior [2]; Tércio de Freitas Paulo [3]; Eduardo Henrique Silva de Sousa [4]; Luiz Gonzaga de França Lopes [5]
[1] UFC (Universidade Federal do Ceará); [2] Laboratório de Bioinorgânica / Departamento de Química Orgânica e Inorgânica / Universidade Federal do Ceará; [3] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica; [4] UNIVERSIDADE FEDERAL DO CEARÁ; [5] Universidade Federal do Ceará

The cis-[Ru(bpy)2(1-meimN)(4-pyCOH)](PF6)2 complex was synthesized and characterized. When irradiated, the complex releases the ligand 4-pyCOH, being promising in photonic therapies.

SÍNTESE, CARACTERIZAÇÃO E ESTUDO FOTOLUMINESCENTE DE COMPLEXO- Eu(DBM)3.NTZ - (NTZ=NITAZOXANIDA)

https://proceedings.science/p/120168

Gabriel Prazeres Usêda [1]; Jorge Fernando Silva de Menezes [2]; Suellen Maria Valeriano Novais [2]; Andrei Marcelino Sá Pires Silva [2]; José Gabriel Santos Barbosa [2]
[1] UFRB; [2] Universidade Federal do Recôncavo da Bahia
Atualmente, tem se estudado um grande número de compostos de coordenação com ligantes orgânicos, entre estes estão os complexos de íons lantanídeos com -dicetonas e ligantes mistos, que podem atuar como dispositivos moleculares conversores de luz (DMCL), absorvendo fortemente radiação no ultravioleta e emitindo no visível. O interesse nesses materiais deve-se as suas diversas aplicações tecnológicas tais como: marcadores luminescentes em fluoroimunoensaios, mini lasers, fósforos para lâmpadas fluorescentes, detectores solares e microdispositivos

eletroluminescentes, etc. Assim sendo, o presente trabalho tem como objetivo a síntese e estudo fotoluminescente de um novo material envolvendo a combinação de um precursor do tipo, Eu(DBM)3.2H2O (DBM=dibenzoilmetanato), que tem a molécula de água (oscilador de alta frequência inibidor de emissão) substituída pelo pró-fármaco nitazoxanida (NTZ-figura 1). A reação do sal de lantanídeo hidratado com o ligante NTZ originou um complexo sólido, Eu(DBM)3.NTZ, em forma de pó amarelo, com perfil cristalino fortemente luminescente sob excitação UV. Analisando os espectros vibracionais na região do infravermelho (IV) pode-se constatar a evidência da ocorrência de coordenação envolvendo o íon európio, Eu3+. O espectro IV de NTZ, revela quatro bandas de estiramento características em 3357, 1774, 1661 e 1604 cm-1 atribuídas para éster ν(NH), ν(C = O), ν(C = O) amida e ν(C = N) tiazol. Após a quelação, o modo ν (NH) é deslocado para comprimentos de onda mais altos, o que elimina o envolvimento do grupo funcional -NH- na esfera de coordenação do íon Eu3+. Alternativamente, os modos ν(C = O) amida e ν(C = N) tiazol são deslocados para comprimentos de ondas menores que podem ser tomados como uma evidência da natureza bidentada da NTZ. O modo ν(C = O) amida é observado em 1646, 1648 e 1644 cm-1 , enquanto o ν(C = N) tiazol é sobreposto às vibrações ν(C = C) gerando uma nova banda de combinação no intervalo de 1553-1550 cm-1 . A banda do éster ν(C = O) é observada na região de 1765-1763 cm-1, o que sugere a participação do grupo -COO- nas interações intra ou intermoleculares com as moléculas vizinhas. O espectro de emissão obtido a 298K na faixa de 500-720 nm, com o monitoramento da excitação em torno de 366nm mostra bandas correspondentes às transições do estado excitado 5D0 para o fundamental 7FJ (J = 0, 1, 2, 3 e 4). A amostra apresenta a emissão, 5D0→7F0, indicando que o centro metálico pode possuir uma simetria Cnv, Cn, ou Cs. A única linha de emissão na transição 5D0→7F0 em 580 nm pode ser atribuída à existência de um único sítio de simetria em torno do íon Eu3+. A característica proeminente notada no espectro de emissão é a alta intensidade da transição 5D0→7F2, em torno de 612nm (a maior intensidade da transição 5D0→7F2 em relação à 5D0→7F1, indica a ausência de centro de simetria). Os resultados iniciais apontam para alternativas de novas combinações envolvendo ligantes de baixo custo para possível fabricação de novos materiais luminescentes, ou seja, a possibilidade da arquitetura de dispositivos fotoluminescentes baratos e com alta eficiência quântica.

Spherical Particles of Ruby by Aerosol Pyrolysis

https://proceedings.science/p/120575

Euzane Gomes da Rocha [1]; José Maurício Almeida Caiut [1]
[1] Universidade de São Paulo (USP)

Ruby is a useful material in strategic areas as photonics and medical
A new methodology was used for synthesis of ruby particles
Particles showed high chemistry stability and intensity high luminescence

SYNTHESIS AND CHARACTERIZATION OF ACTIVATED CARBON FROM SOURSOP SEED (annona muricata L.)

https://proceedings.science/p/119944

Mísia Hadassa Silva Félix [1]; Ivoneide de Carvalho Barros [2]; Rômulo Pereira de Almeida [2]
[1] Laboratório de Química de Materiais - LAQUIMAT, Departamento de Química, Universidade Federal Rural do Pernambuco.; [2] Universidade Federal Rural de Pernambuco

Reuse of soursop seed residue for the production of activated carbon via chemical activation with H3PO4 and ZnCl2.
Characterization of the seed and coal from the residue.

SYNTHESIS AND CHARACTERIZATION THIADIAZOLE-PALLADIUM (II) COMPLEX: STRUCTURAL ASPECTS

https://proceedings.science/p/119874

Eduardo Francisco da Silva Guimarães [1]; Luana Giusto [2]; Eduardo Tonon de Almeida [2]
[1] Universidade Federal de Alfenas-MG/ Instituto de Química; [2] Universidade Federal de Alfenas

Synthesis and characterization of a new Palladium (II) complexes with thiadiazole as the ligand. Synthesis from reaction planning. The complex was characterization by IR and thermal analysis (TG-DTA).

Synthesis and crystalline structure of a new Eu3+ complex

https://proceedings.science/p/120529

Fernanda Sodré Rodrigues [1]; Maryene Alves Camargo [1]; Hevelin Balbino de Almeida [1]
[1] Universidade de Brasília

A new complex of europium was synthesized and its crystalline structure resolved. The complex displays one Eu3+ ion, four molecules of the picolinic acid and one Na+ ion in its coordination sphere.

Synthesis and photoluminescent properties of novel lanthanide complexes containing carboxylate ligands

https://proceedings.science/p/119751

Ercules Teotonio [1]; Iana V.s. Oliveira [1]; Joaldo G. Arruda [1]; Tássio Max dos Anjos Martins [1]; Hermi Brito [2]; Israel Ferreira da Costa [1]
[1] Universidade Federal da Paraíba; [2] Universidade de São Paulo

Novel lanthanide carboxylate complexes were synthesized and characterized. The thermogravimetric properties were investigated. The intramolecular ligand-to-metal energy transfer processes were studie

Synthesis and spectroscopic characterization of the copper complexes supported by phenoxy-imine ligands with pendant O and S-donor groups

https://proceedings.science/p/120502

Tamara dos Santos Machado [1]; Danielle Tapia Bueno [1]; Ianka Jacondino Nunes [1]; Adriana Castro Pinheiro [1]
[1] Universidade Federal de Pelotas

Two new copper complexes containing phenoxy-imine ligands with pendant O and S-donor groups were synthesized and characterized by spectroscopic techniques.

Synthesis of Carbon Dots from aniline derivatives to evaluate the effect of substituents on photophysical and structural properties.

https://proceedings.science/p/120180

Ledja Brittes de Oliveira Davi [1]; Cintya D'Angeles do Espírito Santo Barbosa [2]; Dimas José da Paz Lima [3]
[1] Universidade Federal de Alagoas / Universidade Federal de Alagoas; [2] Universidade Federal de Alagoas; [3] UFAL

Synthesis of C-dots in water;
The C-dots were successfully obtained;
Characterization by spectrofluorescence and structural;
Influence of substituents on photophysical properties were analyzed.

Synthesis of compounds derived from 2-(4-hydroxyazobenzene)benzoic acid(HABA).

https://proceedings.science/p/120423

Vinicius Flores da Silva [1]; Izilda A. Bagatin [1]
[1] Universidade Federal de São Paulo

Developing new sensors is rising due to contamination of the environment with toxic species. The focus is on achieving molecules that could perform sensing ability for cations and anion species.

Synthesis, characterization, photophysics and CT-DNA interaction studies of a novel polypyridyl Ruthenium(II) coordination compound

https://proceedings.science/p/120151

Pedro Henrique Luciano da Silva [1]; Fabio da Silva Miranda [1]
[1] Universidade Federal Fluminense

Photophysical characterization of a new high luminescent Ru(II) complex (H2O: em = 0.068; em = 0.72 S, CH3CN: em = 0.13; em =1.1 S). DNA interaction studies indicated intercalative interaction.

The influence of the counter-ion on the photophysical features of Eu3+ or Tb3+-based β-diketonate-tetrakis-complexes

https://proceedings.science/p/119632

Ariane Beltrame [1]; Felipe da Silva Manrique Canisares [2]; Airton G. Bispo-Jr [3]; Camila B. M. L. Silva [1]; Sergio A Marques de Lima [4]; Ana Maria Pires [5]
[1] IBILCE - UNESP - SÃO JOSÉ DO RIO PRETO - SP; [2] Instituto de Química - UNESP; [3] UNESP ARARAQUARA - SP; [4] Universidade Estadual Paulista-Unesp; [5] Universidade Estadual Paulista "Júlio de Mesquita Filho"

The luminescence of lanthanide complexes excels within the photonic field due to their broad range of applications such as in organic light-emitting diodes (OLEDs)[1,2], light-emitting diodes (LEDs) and light-converting molecular devices (LCMD).[3] Among such materials, [Ln(β-diketonate)4] - anionic complexes stand out due to the absence of coordination water molecules, the strong absorption of β-diketones within the UV spectral region, the efficient energy transfer to the Ln3+ center and the efficient light emission of the Ln3+ , arising from f-f-like electronic transitions.[4] Yet, the impact of the counter-ion on the photophysical properties of the anionic complex is an issue that must be considered, as previously highlighted for the [Q][Eu(dbm)4] complex (Hdmb = dibenzoylmethane).[4] Therefore, in this study, we investigated the influence of two different counter-ions (Na+ or the caudate Q1+ = didodecyldimethylammonium bromide - C26H56BrN) on the luminescence of the [Q][Eu(dbm)4] or the [Q][Tb(acac)4] (Hacac = Acetylacetone) complexes. The complexes were prepared by mixing the solutions of LnCl3 with the deprotonated β-diketones and the counter-ion, under magnetic stirring at 25°C for 4h. FTIR-ATR and UV-Vis measurements confirmed the successful coordination of the ligands to the respective lanthanide ions. Moreover, the Eu3+ complexes had their structures theoretically optimized by using the LUMPAC package. Under UV excitation, the Eu3+ complexes displayed the typical Eu3+ narrow emission bands within the red spectral region (maximum at 613 nm) arising from the 5D0→7F0-4 electronic transitions, while the Tb3+ complexes exhibit the usual Tb3+ narrow emission bands coming from the 5D4→7F6-2 electronic transitions, with maximum at 547 nm, within the green spectral region. The change of the Na+ counter-ion by the Q1 + one led to an increase of the emission relative intensity in the powder, 5 times more intense to Eu3+ complex and 1.25 to the Tb3+ one. This behavior is due to conformational changes in the structure of the anionic complex, proving that the counter-ion plays an important role on their luminescence. Therefore, the complexes synthesized by using the Q1+ caudate counter-ion are better candidates for several applications such as in LEDs, OLEDs, and LCMD.

The Non-Hydrolytic Sol-Gel Methodology used to Prepare GdVO4 Matrix Doped Er3+:Yb3+

https://proceedings.science/p/119761

Eduardo José Nassar [1]
[1] UNIFRAN

Theoretical studies of Nitrosyl Complex: Mechanisms of NO release

https://proceedings.science/p/120684

Bruna Talia dos Santos Carvalho [1]; Luiz Henrique da Costa Souza [2]; Macário Rodrigues [3]; Vitória Soares [4]; Izaura Cirino Nogueira Diogenes [1]; Francisco Lima [5]; Tércio de Freitas Paulo [1]

[1] Universidade Federal do Ceará - Departamento de Química Orgânica e Inorgânica; [2] UFC (Universidade Federal do Ceará); [3] UNIVERSIDADE FEDERAL DO CEARÁ; [4] Universidade Federal do Ceará; [5] Universidade Estadual do Piauí

Theoretical approach on the mechanism of NO release from nitrosyl ruthenium complexes

Um novo polímero de coordenação 3D de Cu2+ com ligantes mistos N- e O- doadores e uma rede topológica 6-conectada do tipo pcu

https://proceedings.science/p/120506

Carlos Magno Dias da Silva Junior [1]; Talita Valverde Ferreira da Silva [1]; Júlia Bruce Alves [1]; Chris Hebert de Jesus Franco [1]; Maria Clara Ramalho Freitas [2]; Charlane Cimini Corrêa [1]

[1] Universidade Federal de Juiz de Fora; [2] Universidade Federal Rural do Rio de Janeiro

Synthesis of a new 3D coordination polymer. Crystal structure revealed a paddlewheel SBU. There is the formation of a 2D network that is pillared by the hmt ligand forming a 3D network.

Química Medicinal - MED

Molecular Docking of Proposed Inhibitors for a Metalloprotease Associated with Schitosoma mansoni Infection

https://proceedings.science/p/120404

Andrei Silva de Faria Rocha [1]; Arthur Kummerle [1]; Carlos Sant Anna [1]

[1] Universidade Federal Rural do Rio de Janeiro

Metalloproteases are involved in schistosomiasis. Molecular docking with a Schistosoma metalloprotease identified thiosemicarbazones as promising compounds to act as its inhibitors.

(E)-Ethyl-2-cyano-3-(3,5-di-tert-butyl-4-hydroxyphenyl)acrylate (MAT-02) as a Promising Larvicidal Agent Against Aedes aegypti

https://proceedings.science/p/120283

Matheus Gabriel Moura Gomes [1]

[1] Universidade Federal de Alagoas

INTRODUCTION: In general, zoonotic infectious diseases are transmitted to humans through hematophagous insects, such as mosquitoes, flies, and tick-borne. In sense, these viruses are named arthropod-borne viruses. Mosquitoes are vectors of several economically impacting pathogens, such as Dengue (DENV), Zika (ZIKV), and Chikungunya (CHIKV) viruses. These viruses are mainly transmitted by the bite of the infected vector, in this case, mosquitoes from the *Aedes aegypti* and *Ae. albopictus* species. Unfortunately, insecticide utilization has led to the emergence of resistant mosquitoes. **AIMS:** The aims of this work were synthesized α-cyanoester derivatives, perform a larvicidal screening against *Ae. aegypti* larvae, and propose a potential target from *Ae. aegypti* by using docking. **METHODS:** Initially, a set of 132 in-house ligands was virtually screened by using GOLD® v. 5.4.0 to perform docking simulations. In sense, different biological targets from *Ae. aegypti* were utilized, such as kynurenine aminotransferase (PDB: 1YIZ), 3-hydroxykynurenine transaminase (PDB: 6MFB), odorant-binding protein 1 (PDB: 3K1E), odorant-binding protein 22 (PDB: 6P2E), pyruvate kinase 1 (PDB: 6DU6), arylalkylamine *N*-acetyltransferase like 5b (PDB: 5YAG), sterol carrier protein 2 (PDB: 2NBM), glutathione *S*-transferase epsilon 2 – GSTe2 (PDB: 5FT3), and alanine glyoxylate

aminotransferase (PDB: 2HUU). α-cyanoesters (**MAT** compounds) was synthesized by adaption of the methods of Yadav *et al.* All derivatives were characterized by ^{1}H and ^{13}C NMR, HLPC, purity (≥ 96%), and melting point. Then, all compounds were screened toward *Ae. aegypti* larvae. Larvicidal assays were performed in triplicates as described by WHO3 with adaptations by Júnior4 and Fujiwara *et al.*5 In sense, L4-stage larvae were exposed to the compounds solubilized in 330 µL DMSO poured into 100 mL of distilled water. The mortality rate is evaluated after 24 and 48 hours post-treatment. All compounds were tested at 5, 50 and 100 ppm concentrations, and Temephos (3 ppm) and DMSO (330 µL) were utilized as positive and negative controls, respectively. Finally, the effects of compounds were verified by morphological and HPLC analysis of the larvae, post-treatment. **RESULTAND DISCUSSION:** From virtual screening, three α-cyanoesters were selected as promising compounds in this study. In general, these analogs were obtained with satisfactory yield, ranging from 64 to 85%. Additionally, the chemical characterization by ^{1}H and ^{13}C NMR and HPLC was sufficient to confirm these derivatives. The larvicidal assay revealed that the **MAT-02** (3,5-C(CH3)3, 4-OH) demonstrated the best activitie, with mortality value 98.3 at 100 ppm concentration (48h). Moreover, CL50 value was determined for **MAT-02** in triplicate as 12.8 ppm. From the morphological analysis, it was verified that both of these compounds were able to kill larvae during the larva-pupa transition. Considering these results, molecular docking simulations were employed to predict a potential target for **MAT-02** (best), where it was found that the GSTe2 is possibly the biological target involved in its activity. This compound interacts at the same binding for glutathione with Pro14, Leu36, His41, Thr54, Val55, Glu67, His69, Phe108, and Arg112. **CONCLUSION:** All virtual simulations were corroborated by experimental results and also a possible macrobiological target from *Ae. aegypti* and *Ae. albopictus* was identified, being GSTe2. Finally, the compound **MAT-02** was identified as a promising larvicidal agent for designing more potent molecules in the future.

2D QSAR Studies on a Series of Fenarimol Derivatives with Trypanocidal Activity

https://proceedings.science/p/120078

Leonardo Luiz Gomes Ferreira [1]; Anacleto Souza [1]; Adriano D. Andricopulo [1]
[1] Physics Institute of São Carlos (IFSC), University of São Paulo (USP)

A robust and predictive Hologram Quantitative Structure-Activity Relationship (HQSAR) model was developed for a series of 52 fenarimol derivatives with anti-Trypanosoma cruzi activity.

A novel disulfide-imide strategy for the intracellular delivery of antibiotic drug linezolid mediated by cell penetrating peptide P14LRR

https://proceedings.science/p/120590

Jean Chmielewski [1]; Paulo Pitasse [2]; Marco Edilson Freire de Lima [2]
[1] Purdue University; [2] Universidade Federal Rural do Rio de Janeiro

Functionalization of antibacterial drug linezolid via imide linkage. Synthesis optimization for amino acid Fmoc-PR(Boc)2-OH. Synthesis of peptide-drug conjugate. Kinetic studies for drug release.

Copper(II) complexes and their aroylhydrazone ligands as potential anticancer drugs

https://proceedings.science/p/120676

Jesica Paola Rada Arias [1]; Ana M. Percebom [1]; Nicolás A. Rey [1]; Vincent Corcé [2]; Michèle Salmain [2]
[1] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio); [2] Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université
Novel Cu2(II)-complexes and aroylhydrazonic ligands. DNA interaction studies. Metallation and transmetallation of biological ions. Pyridine-compounds versus phenol-compounds anticancer properties.

Design and synthesis of new hybrids from a 1,2,4-triazole, prepared from piperine, and known nitroimidazolic drugs

https://proceedings.science/p/120355

Afonso Santine Magalhães Mesquita Velez [1]; Douglas Chaves de Alcantara Pinto [1]; Gabriella Calheiros Magalhães [1]; Paulo Pitasse Santos [1]; Débora Decoté Ricardo [1]; Marco Edilson Freire de Lima [1]

[1] Universidade Federal Rural do Rio de Janeiro

Chagas disease (American trypanosomiasis) is a parasitosis caused by the protozoan Trypanosoma cruzi. The vectorial transmission route has the insect known as “kissing bug” (Triatoma infestans) as the main agent. According to WHO data, this parasitosis is part of a group of diseases called neglected tropical diseases, which is the most neglected. Currently, the therapeutic arsenal for the treatment of chagasic patients is very limited, with only two drugs, both of which are nitroheterocyclic derivatives, Nifurtimox and Benzonidazole; These two drugs are very limited and inefficient in the chronic phase of the disease, causing severe side effects, Our research group reported the trypanocidal effects of natural piperine and several of its derivatives. Recently, piperine’s heterocyclic derivatives bearing a 1,2,4 triazolic ring were described as having important anti-T. cruzi effects. The molecular planning developed here in was based on the molecular hybridization of 1,2,4-triazole core from piperine and the nitroimidazole portion of the know nitroheterocyclic drugs benzonidazole and metronidazole, present in both with well-described antiparasitic activity; aiming to enhance its activity through the synthesis of two novel hybrids that can act through two distinct mechanisms of action on parasite’s cell. The new hybrids were prepared in good yields from natural piperine and and they were characterized by the methods of analysis; highlighting the main signals signals of the NMR 1H and 13C spectra, which confirm the synthesis of these hybrids, in δ 3,62 ppm (t, 2H); δ 45,22 ppm and δ 3,63 ppm (t, 2H); δ 48,59 ppm which characterize the bond formed between CH2 and Sulfur for hybrids. The assessment of toxic effects of the novel hybrids against T. cruzi amastigotes (Tulahuen C2C4 LacZ strain) is underway in our laboratory.

Design and Synthesis of Novel Acrylamide Derivatives as Promising Inhibitors of E3-E2-E1-Glycoproteins Complex from Chikungunya Virus

https://proceedings.science/p/119912

Gabriel Felipe Silva Passos [1]; Matheus Gabriel Moura Gomes [2]; Thiago Mendonça de Aquino [2]; Joao Xavier de Araújo Júnior [2]; Stephannie Janaina Maia de Souza [2]; João Pedro Monteiro Cavalcante [2]; Elane Conceição dos Santos [2]; Ênio José Bassi [2]; Edeildo Ferreira da Silva-Júnior [2]

[1] Universidade Federal de Alagoas - UFAL; [2] Universidade Federal de Alagoas

Zoonotic diseases account for billions of cases of human illness and thousands of deaths around the world, constituting a global public health problem. Frequently, infectious diseases caused by CHIKV are characterized by inflammation and pain of the musculoskeletal tissues, which often these are accompanied by swelling in the joints, resulting in cartilage damage. Currently, there are no licensed vaccines or chemotherapeutic agents able to prevent or treat CHIKV infections. Several acrylamide compounds have been synthesized in different anti-CHIKV studies, where they have demonstrated promising anti-CHIKV activity. Recently, our research group has developed acrylamides with potential anti-CHIKV activity. In sense, **LQM334** was found to be active against infected *Vero E6* cells by CHIKV, with an inhibition value of 81% at 40 µM concentration. In addition, **LQM334** was able to reduce the percentage of CHIKV-positive cells from 74.07 to 0.88%, 48h post-treatment on flow cytometry. Furthermore, molecular docking simulations revealed that this acrylamide derivative possibly performs its antiviral effect by interaction with E3-E2-E1-glycoproteins complex(PDB: 3N41), acting as an entry inhibitor. Now, we have performed rational modifications at the **LQM334** structure in order to improve the anti-CHIKV activity. In sense, all structural modifications (**LQM347-351**) were previously analyzed by molecular docking simulations, where only compounds with FitScoreChemPLP ≥ 46.05 were synthesized and screened for cell viability and antiviral assays. From viability assays, it was observed that **LQM349** and **LQM351** exhibit significant cytotoxic effects at 40 µM concentration, after 48h. Thus, both of these analogs were not evaluated upon infected *Vero E6* cells by CHIKV (antiviral assay). In contrast, **LQM347**, **LQM348**, and **LQM350** demonstrated good tolerance in cytotoxic assays and then these were screened for their anti-CHIKV activities. In sense, it was found that these compounds showed inhibition percentage higher than 50% at 40 µM concentration, after 48 h (CHIKV killed 55% of cells). Finally, molecular docking simulations revealed that **LQM347**, **LQM348**, and **LQM350** are able to interact at the same binding site for **LQM334**, suggesting that these compounds also could act as entry inhibitors.

Design and synthesis of novel alfa-mangostin-nitroimidazole hybrids with toxic effects on amastigotes of Trypanosoma cruzi

https://proceedings.science/p/120350

Douglas Chaves de Alcantara Pinto [1]; paulo pitasse [1]; Gabriella Calheiros-Magalhães [1]; Afonso Santine Magalhães Mesquita Velez [1]; Marco Edilson Freire de Lima [1]; Debora Decoté-Ricardo [1]

[1] Universidade Federal Rural do Rio de Janeiro

alfa-Mangostin (MGT) is the main product isolated from the the fruit pericarp of Garcinia mangostana. This xanthone exhibits important toxic effects on T. cruzi amastigotes. We describe herein the synthesis of new hybrid derivatives of MGT and nitroimidazoles using click reaction as the key-step. Toxic effects on intracellular amastigotes of T. cruzi (Tulahuen C2C4 LacZ).

Design, synthesis and biological assessment of a series of cationic amphiphilic peptides with selective antibacterial activity

https://proceedings.science/p/120583

Paulo Pitasse [1]; Debora Decoté-Ricardo [1]; Jean Chmielewski [2]; Marco Edilson Freire de Lima [1]

[1] Universidade Federal Rural do Rio de Janeiro; [2] Purdue University

Solid-supported synthesis of peptides. Secondary structure investigation via circular dichroism. Antibacterial activity (MIC and mode of action). Cytotoxicity against J774-A1 cells and human RBC.

Development of direct method for monitoring 5x0092-deoxy-5x0092-methylthioadenosine phosphorylase activity and inhibitors screening

https://proceedings.science/p/119520

Juliana Gomes Rodrigues [1]; Quezia Bezerra Cass [1]; Marcela Moraes [2]

[1] Universidade Federal de São Carlos; [2] Universidade Federal Fluminense

Development of liquid chromatography method for direct monitoring of 5'-deoxy-5'-methylthioadenosine phosphorylase enzymatic activity without the use of a coupled assay.

Development of Trypanosoma brucei sirtuin-2 inhibitors by fragment optimisation

https://proceedings.science/p/120336

Renan Augusto Gomes [1]

[1] Faculdade de Ciências Farmacêuticas - USP

Discovery of novel Zika virus NS3 protein inhibitors through the integration of docking, machine learning models and experimental evaluation

https://proceedings.science/p/120687

Bruna Katiele de Paula Sousa [1]; Melina Mottin [2]; Jean Bernatchez [3]; Nathalya Mesquita [4]; Zhe Zhu [3]; Jeremy Rich [3]; Alex E. Clark [3]; Kimberley Zorn [5]; Daniel Foil [5]; Geraldo Rodrigues Sartori [6]; Aline O. Albuquerque [6]; João Herminio Martins [6]; Bruno Neves [7]; Eugene N Muratov [8]; Alexander Perryman [9]; Glaucius Oliva [4]; Jair Siqueira-Neto [3]; Sean Ekins [5]; Carolina Andrade [1]

[1] Laboratory of Molecular Modeling and Drug Design (LabMol) / Faculty of Pharmacy / Federal University of Goiás; [2] Federal University of Goiás; [3] University of California; [4] Institute of Physics of São Carlos, University of São Paulo, São Carlos, SP, Brazil; [5] Collaborations Pharmaceuticals, Inc., Raleigh, NC, USA; [6] Fundação Oswaldo Cruz; [7] Universidade Federal de Goiás; [8] University of North Carolina - University of North Carolina at Chapel Hill, USA.; [9] Department of Pharmacology, Physiology and Neuroscience, Rutgers University–New Jersey Medical School, Newark

Virtual screening for ZIKV NS3 proteíns prioritized 59 promising virtual hits. 16 compounds inhibited ZIKV in cells and enzymatic assays showed that one compound inhibited ZIKV NS3 protease.

Evaluation between biological activity and binding energy provided by docking programs for benzylidene-acrylohydrazide derivatives in CHIKV nsP2 protease

https://proceedings.science/p/119767

Larissa Silva Muniz [1]; Isabela de Oliveira Estrela [1]; Samuel Silva da Rocha Pita [1]

[1] Universidade Federal da Bahia

O vírus Chikungunya (CHIKV), membro da família Togaviridae e do gênero alfavírus, é um arbovírus emergente que se apresenta como um problema de saúde pública em todo o mundo. Classificada pela OMS como uma doença tropical negligenciada, a febre causada pelo CHIKV (CHIKF) é caracterizada por uma poliartalgia intensa e incapacitante. Até o momento ainda não há tratamento antiviral específico, diante deste cenário, a busca por fármacos anti-CHIKV é urgente. A proteína não estrutural 2 (nsP2) é considerada um alvo terapêutico devido à sua atividade de protease essencial para a replicação viral. Gianciotti e colaboradores (2018) sintetizaram uma série de derivados benzilideno-acrilhidrazida que mostraram atividade anti-CHIKV (EC50). Analisando suas propriedades farmacocinéticas e toxicológicas por diversas ferramentas, descobrimos que eles: i) seguem a regra de Lipinski, portanto podem apresentar boa biodisponibilidade oral; ii) são capazes de penetrar no SNC e iii) não são hepatotóxicos. A fim de entender melhor seu comportamento anti-CHIKV, fizemos o acoplamento desses compostos frente à nsP2 (*apo*, código PDB: 3TRK), usando funções de pontuação distintas (AutoDock 4.2, AutoDock Vina e GOLD), com o objetivo de verificar qual deles apresentava a melhor correlação entre atividade biológica e a energia de acoplamento. Os resultados mostraram que o GOLD (através da função de classificação PLP) classifica 50% dos compostos mais ativos (5,59 < -logEC50 < 4,53) entre as melhores energias, seguido pelo Autodock 4,2 (43%), Vina (29%) e o GOLD, empregando a função ChemScore (21,5%). No entanto, o AutoDock 4.2 obteve uma menor taxa de falsos-positivos (8%) em relação à função PLP (28%), o que nos levou a escolher o AutoDock 4.2 para analisar o modo de interação. O composto 51 obteve a melhor energia (-8,75 kcal/mol) interagindo através de ligações hidrogênio com os resíduos: ALA-1010, ASN-1011, LYS-1016 e ASN-1082, os quais auxiliam na ligação do substrato da nsP2. Além disso, a série de compostos 23 (a - e) foram bem classificados em todos os programas, embora sejam menos ativos. Assim, nossos resultados ajudam a entender a relação estrutura atividade para os derivados de benzilideno-acrilhidrazida com o objetivo de se planejar um inibidor com ação na nsP2 de CHIKV.

Fatty-dihydropyridines: docking calcium channel and antihypertensive activity

https://proceedings.science/p/120116

Marcelo Montes D'Oca [1]

[1] Universidade Federal do Paraná

Formulações à base de lipídios influenciam os parâmetros de absorção de parabenos através do ensaio PAMPA pele

https://proceedings.science/p/120515

Ana Paula Ruani [1]; Bruna Ribeiro Souza [2]; Gustavo Micke [2]

[1] Departamento de Química / Centro de Ciências Físicas e Matemáticas / Universidade Federal de Santa Catarina; [2] Universidade Federal de Santa Catarina

Parabens were capable of permeating the artificial membrane and their retention decreased in the presence of the formulation 1.

Hotspot conservation across open/closed protein pairs: early steps towards successful docking studies with APO structures.

https://proceedings.science/p/120009

Pedro Sousa Lacerda [1]; Kleiton Luís de Oliveira Souza [2]; Marcelo Castilho [1]

[1] Universidade Federal da Bahia; [2] Universidade Federal da Bahia, Faculdade de Fármacia, Departamento de Medicamentos

Druggable sites are more conserved than consensus sites during the transition from APO to HOLO. The conservation of druggable sites can assist in the selection of APO proteins for molecular docking.

In vitro biological evaluation of novels phthalide-thiazole derivates against leishmania spp.

https://proceedings.science/p/119576

Fabiano Amaro de Sousa [1]; Aline Santos [2]; Juliana Conceição [3]; Ignes Regina dos Santos [4]; Mabilly Holanda [5]; Valéria Rêgo Alves Pereira [6]; Ana Cristina Leite [7]

[1] UNINVERSIDADE FEDERAL DE PERNAMBUCO; [2] FIOCRUZ/UFPE; [3] UFPE/PRGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIAS FARMACÊUTICAS; [4] UFRPE/PROGRAMA DE PÓS-GRADUAÇÃO EM QUIMICA; [5] DEPARTAMENTO DE FARMÁCIA / Centro de Ciências da Saúde / UNIVERSIDADE FEDERAL DE PERNAMBUCO; [6] FIOCRUZ-UFPE; [7] UFPE/PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIAS FARMACÊUTICAS

The biological activity of the novels compounds was tested against leishmania amazonensis and infantum. As results, three showed activity against promastigote form and four against amastigote form

INDOL-THIAZOL DERIVATIVES: DNA INTERACTION AND DOCKING STUDIES

https://proceedings.science/p/120391

Franciane Gonçalves dos Santos [1]; Amélia Galdino Ribeiro [2]; Josival Emanuel Ferreira Alves [3]; Keriolaine Lima dos Santos [4]; Jamerson Ferreira de Oliveira [2]; Maria do Carmo Alves de Lima [2]; Túlio Couto [5]; Paulo Henrique Menezes [6]

[1] Universidade Federal de Pernambuco-UFPE/ Departamento de Química Fundamental-DQF; [2] Universidade Federal de Pernambuco - UFPE/ Departamento de Antibióticos; [3] Universidade Federal de Pernambuco - UFPE/Laboratório de Imunopatologia Keizo Asami (LIKA),; [4] Universidade Federal de Pernambuco - UFPE/Departamento de Antibióticos; [5] Unidade Acadêmica de Belo Jardim; UFRPE; [6] Universidade Federal de Pernambuco-UFPE/ Departamento de Química fundamental

Agents that act on DNA are object of study in the development of chemotherapic agents. In this context, seven indole-thiazoles were evaluated in silico and in vitro as DNA ligands.

Interação de pisosterol e derivados com DNA explorando estudos biofísicos - relação com atividade antiproliferativa

https://proceedings.science/p/120563

Karlly Thayanny de Oliveira Pimentel [1]; Ari Souza Guimarães [1]; Maria da Conceição Ferreira de Oliveira [2]; Paulo Sousa Júnior [2]; Fátima Oliveira [2]; Claudia Pessoa [2]; Josué Carinhanha Caldas Santos [3]; Isis Figueiredo [1]

[1] Universidade Federal de Alagoas; [2] Universidade Federal do Ceará - UFC; [3] Universidade Federal de Alagoas

DNA is a biological target in cancer studies, and pisosterol, which was the most active against different strains of human cancer cells, interacts with it via groove and high binding constant.

Machine learning models for predicting the transmission-blocking activity of compounds against Plasmodium sp.

https://proceedings.science/p/119975

Sabrina Silva Mendonça [1]; Joyce Villa-verde Bastos Borba [2]; Bruno Neves [1]; Juliana Calit Paim [3]; Richard Eastman [4]; Daniel Youssef Bargieri [3]

[1] Universidade Federal de Goiás; [2] Universidade de Campinas; [3] Universidade de São Paulo; [4] National Institutes of Health

Malaria remains a public health issue, with about 228 million cases and 500.000 deaths annually.1 Evolution of parasite strains resistant to all known classes of antimalarial drugs urges the need for novel lead compounds, including to block transmission.2 Aiming to discover new antimalarial drugs, we developed robust and predictive machine learning models for predicting transmission-blocking activity of compounds against Plasmodium berghei. Initially, a high throughput screening collection of 6636 compounds with experimental transmission blocking data was curated and standardized according to best practices of Fourches and co-workers.3 Then, categorical machine learning models combining ten fingerprints (AtomPair, Avalon, Dragon, FeatMorgan, Layered, MACCS, Morgan, Pattern, RDKit, and Torsion) with two machine learning methods (Random Forest and Naïve Bayes) were developed following the best practices of predictive modeling.4 As a result, we have obtained statistically predictive models, with CCR, Sensitivity, and Specificity values ranging between 0.79–0.84. Subsequently, the most predictive model (combining Random Forest and Torsion fingerprints) was used in a virtual screening campaign along with two other models (asexual stages of P. falciparum W2 and 3D7 strains) previously developed in our laboratory.5 Using these models, we prioritized 40 compounds for further in vitro testing against asexual and sexual stages of Plasmodium spp.

Modelagem Molecular Aplicada à Descoberta de Candidatos a Inibidores de Metaloprotease de Trypanosoma Cruzi

https://proceedings.science/p/120606

Alessandra Gonçalves [1]; Arthur Kummerle [1]; Carlos Sant Anna [1]
[1] Universidade Federal Rural do Rio de Janeiro

Analysis of compounds as candidate inhibitors of T. Cruzi metalloprotease, using docking and semiempirical calculations. The results indicate that some compounds can interact effectively with the enzyme.

Molecular docking and fluorescence based enzymatic inhibition assay: a study of T. cruzix0092s CYP51 inhibition by heterocyclic compounds

https://proceedings.science/p/119664

Larissa Castro [1]; Aurea Echevarria [1]; Demian Rocha Ifa [2]; Marco Lima [1]; Carlos Sant Anna [1]
[1] Universidade Federal Rural do Rio de Janeiro; [2] York University - Toronto/CA

The T. cruzi CYP51 inhibition activity of heterocyclic compounds was evaluated by docking and a fluorescence-based enzyme inhibition assay, with promising results for triazole piperine derivatives.

Molecular Docking and Larvicide and Toxicological Evaluation of Ethyl p-chlorocinnamate against A. aegypti, S. lycopersicum and L. sativa

https://proceedings.science/p/120081

Saraliny Bezerra França [1]; Edeildo Ferreira da Silva - Júnior [2]; Cenira Monteiro de Carvalho [2]; Maria Ester de Sá Barreto Barros [2]; Josealdo Tonholo [2]; Dimas José da Paz Lima [2]
[1] Universidade Federal de Alagoas/ Instituto de Química e Biotecnologia; [2] Universidade Federal de Alagoas

Ethyl *p*-chlorocinnamate has proven to be a good larvicide agent with low toxicity to some plants. Its potential is due to the inhibiting of AChE, according to the molecular docking study.

New hybrid 1,4-naphthoquinones as potential anti-T. cruzi agents

https://proceedings.science/p/120327

Alcione Silva de Carvalho [1]; Fernando de Carvalho [1]; Vitor Ferreira [1]
[1] Universidade Federal Fluminense

Chagas disease (CD) is still one of the most concerning public health problems in 21 Latin American countries.1 Migration and specific modes of transmission have led to CD spreading beyond its natural geographical boundaries and becoming a global issue. The current treatment of CD is based on the use of two drugs, nifurtimox (Nfx) and benznidazole (Bnz), which present limited efficacy in the chronic stage of the disease and toxic side effects.1 In Brazil, only Bnz is used for treatment of CD.1 Our research group has achieved promising results with 1,4naphthoquinone derivatives have good activity against T. cruzi through an oxidative process leading to its death (Figure 1).2,3,4 Continuing our study, we present in this work the synthesis of novel 1,4-napthoquinones and their trypanocidal, and toxicological evaluation. These compounds were designed by hybridization molecular of quinones system and 1,2,4-triazole nucleus, that are also present in different anti-T. cruzi substances.1,4,5 The methodologie employed for the synthesis of the novel hybrids was from nucleophilic substitution reaction of 1,4- naphthoquinone with 3-amino-5-R-1,2,4-triazole. It consist of three steps, this being of great relevance since it is about designing a new leader for a neglected disease. The final products will sent to the in vitro test in trypomastigotes and amastigote forms of T. cruzi in Y strain. They will be sent also to cytotoxicity in human blood cells. With the results of biological and toxicological activities, it is expected to achieve the goal of the work in obtaining a more active and / or less cytotoxic substance than Nfx and Bnz drugs. References: [1]WHO report on neglected tropical diseases; https://www.who.int/chagas/en/; [2]Lara, L.S et al 2018 Europ J Med Chem, 144, 572-581; 3Diogo, E.B.T. et al 2013 Bioorg Med Chem 21, 6337-6348; 4Ferreira, S.B. et al 2010 Rev Virt Quím, 2, 140-160; 5Salomao, K., et al 2016 Curr. Top. Med. Chem. 16, 2266-89.
Acknowledgments CAPES - Finance Code 001; FAPERJ; PNPD-UFF, CNPq and Fiocruz.

New piperaquine derivatives with potential activity anti-P. falciparum

https://proceedings.science/p/119725

Lívia de Melo Feitosa [1]; Luma Carolina Figueredo da Silva [2]; Mayara Ferreira [1]; Maria de Lourdes Garcia Ferreira [2]; Luiz Carlos da Silva Pinheiro [2]; Núbia Boechat Andrade [2]

[1] Fiocruz; [2] Síntese de Fármacos / Farmanguinhos / Fiocruz

Four piperaquine derivatives were synthesized in overall good yields 28-45%. The anti-P. falciparum activity of these substances is being evaluated.

New pyrazolopyrimidine and triazolopyrimidine derivatives with potential activity anti-P. falciparum

https://proceedings.science/p/119727

Lívia de Melo Feitosa [1]; Gustavo Peixoto Machado [2]; Gabriel Matheus dos Santos de Araujo [2]; Maria de Lourdes Garcia Ferreira [2]; Larissa Guimarães Oliveira [2]; Luiz Carlos da Silva Pinheiro [1]; Juliana Oliveira de Souza [3]; Anna Aguiar [3]; Rafael Victorio Carvalho Guido [4]; Núbia Boechat Andrade [5]

[1] Fiocruz; [2] Síntese de Fármacos / Farmanguinhos / Fundação Oswaldo Cruz; [3] Universidade de São Paulo; [4] Instituto de Física de São Carlos - USP; [5] Fundação Oswaldo Cruz

Eight pyrazolopyrimidine and triazolopyrimidine derivatives were synthesized in 12-30% overall yield and in vitro evaluated against P. falciparum. Compound 13 was the most potent derivative.

Novel 3-nitro-1,2,4-triazole derivatives with potent activity against Trypanosoma cruzi in an intracellular model

https://proceedings.science/p/119891

Cheyene Almeida Celestino Menozzi [1]; Frederico Silva Castelo Branco [2]; Rodolfo Rodrigo Florido França [2]; Policarpo Sales Junior [2]; Silvane Maria Fonseca Murta [2]; Álvaro José Romanha [2]; Nubia Boechat [2]

[1] Fundação Oswaldo Cruz/ Farmanguinhos/ Departamento de Síntese de Fármacos, LASFAR / Instituto de Ciências Biomédicas, UFRJ; [2] Fundação Oswaldo Cruz

Five derivatives were synthesized in overall good yields (9-45%). These proved to have a good absorption profile in silico and showed high potency against Trypanosoma cruzi, higher than benznidazole.

Oxidação de botriosferana, uma ß-glucana com potencial atividade antiviral contra dengue e herpes

https://proceedings.science/p/120550

Flávia Deduch [1]; Marcelle de Lima Ferreira Bispo [1]; Aneli Barbosa [1]; Alexandre Orsato [1]

[1] Universidade Estadual de Londrina

Oxidation of a fungal β-glucan as the first step to obtain a heparan sulfate-like polysaccharide with potential antiviral activity against dengue and herpes simplex viruses.

Preparation of anionic polysaccharides and their antidengue activity

https://proceedings.science/p/120682

José Louzinho Lopes [1]; Vinicius Seiki Takemura Quinteiro [2]; Maria Laura Darido [2]; Elisa Vicente Ribelato [2]; Aneli Barbosa [3]; Ligia Carla Faccin Galhardi [2]; Alexandre Orsato [3]

[1] Universidade Federal do Rio Grande de Sul; [2] Universidade Estadual de Londrina; [3] Departamento de Química / Centro de Ciências Exatas / Universidade Estadual de Londrina

The anionic glucan possess the same anionic groups as heparan sulfate, the host receptor of dengue virus. However, a glucan derivative bearing only sulfate groups exerts higher antidengue activity.

PyAutoFEP: an automated Python tool for setup and analysis of FEP calculations in GROMACS

https://proceedings.science/p/119810

Rafaela Ferreira [1]; Luan Carvalho Martins [1]; Elio Cino [1]
[1] UFMG

Relative binding free energy (RBFE) calculations for small molecules are becoming commonplace. RBFE can be used to predict relative affinities of a series of ligands to a biological target, and, thus, be used to guide optimization in drug discovery campaigns. Free Energy Perturbation (FEP) using molecular dynamics (MD) to simulate non-physical transformations between ligand pairs are among the techniques most extensively used for RBFE prediction. To achieve the high accuracy and speed needed for such predictions to be useful, FEP calculations must use highly optimized MD code, enhanced sampling techniques, and modern force fields. Current hardware allows for hundreds of perturbations to be routinely simulated; however, automation of the setup process is crucial. Here, we report PyAutoFEP, a tool to automate RBFE calculations using FEP. PyAutoFEP is flexible, allowing the user to control over most of the program options, and complete, aiding users through the whole process. PyAutoFEP is composed of three parts: a perturbation map generator, a hybrid topology builder, and an analysis module. PyAutoFEP is opensource, and can be downloaded at GitHub. Three types of perturbation maps can be generated: star maps, wheel maps, and optimal maps. Optimal maps are generated by a modified Ant Colony Optimization, which minimizes the number of perturbed atoms, the distance between two nodes, and the number of perturbations, optionally making a map with cycle closures. The main module converts individual ligand structures and topologies into a hybrid topology, prepares a protein-ligand complex, solvates and add counter ions to it. The hybrid topology is guided by the maximum common structure between the molecules, and multiple force fields can be parsed. PyAutoFEP allows use of arbitrary λ scaling factors for charged and Van der Waals interactions and for A and B end states. Finally, the tool prepares scripts for executing the perturbation. The ΔΔG is estimated by either Bennet Acceptance Ratio (BAR) or Multistep BAR, implemented in alchemlyb. PyAutoFEP includes tools to streamline analysis of ΔΔG convergence, Replica Exchange ratios, and ligand-receptor interactions. To test and validate PyAutoFEP, we used it to study a series of ligands of the Farnesoid X Receptor, an RBFE challenge presented to the community by D3R. We used Amber03/GAFF with AM1BCC charges and Charmm36WYF/CgenFF to predict the ΔΔG of the series with and without enhanced sampling methods. Using Amber03/GAFF, we obtained results par with the reported values using FEP+, and far better than with pure GROMACS free energy code. Results with Charmm36WYF/CgenFF were inferior, showing poorer correlation with experimental data. The use of Hamiltonian Replica Exchange (HREX) or HREX with Solute Scaling did not improve the results.

RAPID ISOLATION OF NUCLEOSIDE HYDROLASE LIGANDS THROUGH LIGANDS FISHING ASSAY

https://proceedings.science/p/120395

Pamella Christina Ortega de Oliveira [1]; Rodrigo Costa da Silva [1]; Millena Santana Ceroullo [1]; Gilberto Alves Romeiro [2]; Maria Cecília B. V. de Souza [1]; Fernanda da Costa Santos Boechat [1]; Luzineide Tinoco [3]; Quezia Bezerra Cass [4]; Marcela de Moraes [1]
[1] Universidade Federal Fluminense; [2] Universidade Federal Fluminense / Instituto de Química / Departamento de Química Orgânica; [3] Universidade Federal do Rio de Janeiro; [4] Universidade Federal de São Carlos

An affinity-based assay was developed for the screening of ligands of Nucleoside Hydrolase from Leishmania donovani (LdNH). The binders were selectively isolated and identified by ESI-HRMS.

SÍNTESE DE DERIVADOS AZÓLICOS COM POTENCIAL ATIVIDADE ANTINEOPLÁSICA

https://proceedings.science/p/120284

Karoline Chagas Lisboa Aboud [1]; Claudia Pessoa [2]; Marcus Souza [1]; Thatyana Vasconcelos [3]; Claudia Regina Brandão Gomes [1]; Victor Facchinetti Luz [1]; Tácio Vinício Amorim Fernandes [4]
[1] Fundação Oswaldo Cruz, Instituto de Tecnologia em Fármacos – Farmanguinhos; [2] Universidade Federal do Ceará - UFC; [3] Universidade Federal Fluminense; [4] INMETRO

Seven new thiazoles containing the quinoline moiety were synthesized and assessed against HL60 and K562 leukemia cell lines. All substances have shown remarkable activity against K562 cells (1-2μM)

Síntese de derivados de ácido vanílico como candidatos contra doenças relacionadas ao estresse oxidativo.

https://proceedings.science/p/120446

Carla Cristina Perez [1]; Keoma Keyson Lima Cavalcante [2]

[1] Departamento de Química / Centro de Ciências Exatas / Universidade Estadual de Londrina; [2] Universidade Estadual de Londrina

Synthesis of Vanillic Acid Derivatives as candidates against diseases linked to Oxidative Stress. Compounds that can act as antioxidants and as inhibitors of the enzyme NADPH oxidase.

Síntese de derivados imidazólicos a partir de isatinas e avaliação do potencial anti chagas

https://proceedings.science/p/120265

Gabriel Freitas do Rio [1]; Jan Pierre de Paiva Soares [2]; Aurélio Baird Buarque Ferreira [2]; Gleyton Leonel Silva Sousa [3]; Gabriella Calheiros Magalhães [2]

[1] UFRRJ; [2] Universidade Federal Rural do Rio de Janeiro; [3] Programa de Pós-Graduação em Química / INSTITUTO DE QUÍMICA / Universidade Federal Rural do Rio de Janeiro

The research seeks to synthesize new compounds from the reaction of isatins with aldehydes, and to evaluate their potential anti-chagas.

Síntese de Híbridos Dipirona-AINES, Planejados como Moduladores de Receptores Canabinoides

https://proceedings.science/p/120674

Daniela Rodrigues [1]; Rodolfo do Maia [1]; Carlos Fraga [1]

[1] Universidade Federal do Rio de Janeiro

New hybrids of dypirone and NSAIDs were synthetized and characterized as CB2 cannabinoid receptors inverse agonists with adequate druglike properties.

Síntese e avaliação de naftoimidazóis: potenciais componentes terenósticos fluorescentes

https://proceedings.science/p/120448

Victória Laysna dos Anjos Santos [1]; Arlan Gonsalves [1]; Helinando Pequeno de Oliveira [1]; Cleônia Roberta Melo Araújo [2]

[1] Universidade Federal do Vale do São Francisco; [2] Universidade Federal do Vale do São Francisco/Colegiado de Ciências Farmacêuticas

Synthesis and evaluation of naphthoimidazoles: potencial fluorescent theranostics components. Synthesis and photophysical study of three naphthoimidazoles derived from lapachol.

Structural Biology applied to drug discovery for schistosomiasis

https://proceedings.science/p/120655

Maria Cristina Nonato [1]

[1] Universidade de São Paulo

Structure-activity and mechanism of action of anacardic acid derivatives that inhibit pyocyanin production in P. aeruginosa

https://proceedings.science/p/120064

Marina Sena Mendes [1]; Thamires Froes [2]; Danilo Santana Galvão [2]; Gabriela S. R. H. Cardoso [3]; Thais A. M. Ferreira [3]; Giselle A. Ramos [3]; Luiz A. S. Romeiro [3]; Marcelo Castilho [1]

[1] Universidade Federal da Bahia; [2] Universidade de São Paulo; [3] Universidade de Brasília

Bacterial resistance is a worldwide problem, that has attracted less and less attention from the Big Pharma industry. This contradictory pattern is explained by the fact that bactericidal and bacteriostatic drugs speeds up resistant strain selection. An alternative to overcome this problem is to reduce bacterial virulence without decreasing its cellular viability. Previously, we have shown that AAD bind to PhzD (E.C.3.3.2.15), an enzyme from the pyocyanin biosynthesis pathway in *P. aeruginosa*, with micromolar affinity (LDT10 (3-decyl-phenol) (Kd= 2.8 µM) and decreases pyocyanin production (48,85% at 50mM). In order to gain some insight into the structure activity relationship of this series, others AAD were screened by thermal shift assays (TSA) and further characterized by fluorescence-based assays, with fluorescein labeled PhzD (PhzD-FITC) . Our results suggest that acetylation (LDT12- inactive) or methylation (LDT27 Kd> 1000 µM) of LDT10's OH moiety significantly decreases the affinity to PhzD. A similar trend is observed when a methyl is added to the carboxyl moiety of LDT13 (Kd=0.78 µM) (LDT29 - inactive). Replacement of carboxyl moiety by hydroxy-methyl leads to >50-fold reduction in affinity (LDT197 Kd> 1000 µM) in comparison to LDT13. In addition, the most promising compound (LDT 10) had its mechanism of action investigated. Gene expression analysis, carried out with a *P. aeruginosa* strain bearing a gene reporter system , reveals that LDT10 significantly reduces ($P < 0,0346$) PhzD expression on the exponential phase of bacterial growth (O.D. 1.0), but has no effect over the stationary phase (O.D. 3.0), when pyocyanin is produced. This result supports the hypothesis that LDT10 biological effect is due to enzymatic inhibition of PhzD and gene expression mechanisms.

Syntesis of new hydrazones triazolopyrimidines derivatives as anti-plasmodium agents

https://proceedings.science/p/119918

Marilia Oliva Gandi [1]; Alcione Silva de Carvalho [2]; Juliana Oliveira de Souza [3]; Anna Aguiar [3]; Rafael Victorio Carvalho Guido [4]; Núbia Boechat Andrade [5]

[1] UFRJ/Fiocruz; [2] Universidade Federal Fluminense; [3] IFSC/USP; [4] Instituto de Física de São Carlos - USP; [5] Fundação Oswaldo Cruz

We designed and synthesized forty two novel hydrazones triazolopyrimidines using tool of medicinal chemistry. Twenty two compounds showed anti-P. falciparum activity.

Synthesis and evaluation of potential antitumor of new acridines-thiosemicarbazones derivatives.

https://proceedings.science/p/120198

Gleyton Leonel Silva Sousa [1]; Agnis Pâmela Simões do Nascimento [2]; Lucas Linhares de Locio [2]; LIDIANE GOMES DE ARAÚJO [2]; Miguel Ângelo Santos Pinheiro Segundo [3]; Malu Maria Lucas dos Reis [3]; Ricardo Olímpio de Moura [2]; Arthur Kummerle [4]

[1] Programa de Pós-Graduação em Química / INSTITUTO DE QUÍMICA / Universidade Federal Rural do Rio de Janeiro; [2] Universidade Estadual da Paraíba - UEPB; [3] Universidade Federal de Pernambuco - UFPE; [4] Universidade Federal Rural do Rio de Janeiro

Chemotherapy consists of the most widely used cancer treatment option. DNA is an important pharmacological target; some forms of drug-DNA interaction are possible.

Synthesis and pharmacological effect of N-oxide derivatives with in vivo sterilizing antitubercular activity.

https://proceedings.science/p/120261

Jean Leandro dos Santos [1]

[1] Faculdade de Ciências Farmacêuticas - UNESP Araraquara

In vivo study revealed no-detectable Mycobacterium tuberculosis in the lungs, exhibiting sterilizing effect on treated animals.

Synthesis and Pharmacological Evaluation of 1,5-diaryl-3-amine-1,2,4-triazoles designed as cholinesterase inhibitors for Alzheimerx0092s Disease treatment

https://proceedings.science/p/120201

Lucas Caruso Araujo Bezerra [1]; Daiana Franco [1]; Sabrina Santos [1]; Luciana Azevedo [1]; Nathalia Fonseca Nadur [1]; Bruno Pinheiro [1]; Arthur Kummerle [1]
[1] Universidade Federal Rural do Rio de Janeiro

Regioselective microwave synthesis of new 1,5-diaryl-3-amine-1,2,4-triazoles; Evaluation of cholinesterase inhibition profile aiming at a treatment for Alzheimer's Disease

Synthesis and Pharmacological Evaluation of New 3-(Imidazo[1,2-a]pyridin-2-yl)-coumarins as Cholinesterase Inhibitors

https://proceedings.science/p/120200

Larissa de Almeida Peixoto Ferreira [1]; Felipe Vitório [1]; Daiana Franco [1]; Luciana Azevedo [1]; Arthur Kummerle [1]
[1] Universidade Federal Rural do Rio de Janeiro

Synthesis and pharmacological evaluation of new imidazopydine-coumarins obtained from coumarin-β-ketoesters planned. Preliminary results showed excellent efficacy on inhibition of cholinesterases.

Synthesis of newly substituted isoquinolinesulfonylhydrazones designed as Rho kinase inhibitors for treatment of heart failure and pulmonary hypertension

https://proceedings.science/p/120091

Tadeu Lima Montagnoli [1]; Bianca Santos-Carlos [1]; Bruna Souza Rocha [1]; Jaqueline Soares da Silva [1]; Gisele Zapata-Sudo [1]; Carlos Fraga [1]
[1] Programa de Pós-graduação em Farmacologia e Química Medicinal, Instituto de Ciências Biomédicas, UFRJ

New isoquinolinesulfonylhydrazones designed and characterized as Rho kinase inhibitors in vitro could reduce cardiovascular remodeling in heart failure and pulmonary hypertension.

Synthesis of novel nitroimidazoles with potential activity against Trypanosoma cruzi

https://proceedings.science/p/120789

Carolina dos Reis Farias [1]; Núbia Boechat Andrade [2]; Frederico Silva Castelo Branco [2]; Alcione Silva de Carvalho [3]
[1] Universidade Federal do Rio de Janeiro; [2] Fundação Oswaldo Cruz; [3] Universidade Federal Fluminense

In this work, molecules with nitroimidazolic nucleus with potential activity against Trypanosoma cruzi were synthesized with global yields of 66-95%.

Triazol-derivatives as novel antimalarials.

https://proceedings.science/p/120356

Benedito Matheus dos Santos [1]; Daniel Tadeu Gomes Gonzaga [2]; Fernando de Carvalho [3]; Vitor Ferreira [3]; Célia Regina da Silva Garcia [4]

[1] Department of Clinical and Toxicological Analysis, School of Pharmaceutical Sciences, University of São Paulo, São Paulo, Brazil; [2] UFAR / CCBS / UEZO; [3] Universidade Federal Fluminense; [4] Universidade de São Paulo

The search for new compounds with antimalarial activity is urgent, as resistance to ones in the classical drug, has already been described in more than one continent. Compounds derived from 1,2,3-triazoles are effective against parasites and bacteria. Here, we evaluated the potential antimalarial activity against the human malaria parasite *Plasmodium falciparum* in a culture of fifty-four triazole compounds derived from 1*H*-and 2*H*-1,2,3-triazole. We identified thirty-one compounds with potential antimalarial activity at concentrations in the micromolar order (μM) and IC50 values ranging from 2.80 μM (9) to 29.27 μM (21). Then, we selected some of these compounds to perform the same tests on the PfSR25- strain (knockout for *P. falciparum* G-protein coupled receptor-like, SR25). Our experiences with the PfSR25- strain showed that both compounds with higher antimalarial activity for the 3D7 strain and those with less activity resulted in lower IC50 values for the knockout strain. The cytotoxicity of the compounds was evaluated in human renal embryonic cells (HEK 293), using MTT assays. This demonstrated that the compounds with the highest activity (9, 13, 19, 22, 24, 29), showed no toxicity at the tested concentrations.

Uso de ferramentas in silico para estudos dos Canais Lentos de Cálcio (LPC)

https://proceedings.science/p/120299

Yria Jaine Andrade Santos [1]; Camila Alves de Lima [2]; Juliane Xavier dos Santos [2]; Aurélia Santos Faraoni [1]; Tiago Branquinho Oliveira [2]

[1] Departamento de Farmácia / Centro de Ciências Biológicas e da Saúde / Universidade Federal de Sergipe; [2] Universidade Federal de Sergipe

This study aimed for a searching of new L-type calcium channel antagonists from a natural products database through in silico tools such as docking and virtual screening.

Validation of 20S proteasome model of Leishmania tarentolae for the design of novel antileishmanial drugs

https://proceedings.science/p/120675

Leonardo Simões [1]; Jean Leandro dos Santos [2]; Nailton Monteiro do Nascimento Júnior [1]

[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho" - Campus Araraquara

The 20S proteasome has been explored for the treatment of leishmaniasis. Thus, a validated 20S proteasome model will furnish conditions for the design of novel antileishmanial drug candidates.

Química Orgânica - ORG

Pirazóis 3,5-dissubstituídos como catalisadores para a reação de cicloadição de CO2

https://proceedings.science/p/120609

Gabriel Pereira Portes Cerqueira [1]; Werberson de Almeida Bezerra [2]; Karine Enes [1]; Mara Rubia Costa Couri [1]; Rafael Pavão das Chagas [2]; Jorge Milani [1]

[1] Universidade Federal de Juiz de Fora; [2] Universidade Federal de Goiás

-Metal-free and solvent-free cycloaddition reaction;
-High conversion and selectivity.

1H NMR-based metabolomics as a potential tool for investigation of urinary biomarkers in fishermen exposed to toxic metals in Maceió-AL

https://proceedings.science/p/119653

Jeferson Santana Ursulino [1]; Reginaldo Correia da Silva Filho [1]; Alessandre Carmo Crispim [1]; Raphael S. Pinto [2]; Chiara R. M. Marinho [2]; Josué Carinhanha Caldas Santos [3]; Ana Catarina Rezende Leite [4]; Thiago Mendonça De Aquino [5]

[1] Universidade Federal de Alagoas; [2] Centro Universitário Cesmac - Centro de Estudos Superiores de Maceió; [3] Universidade Federal de Alagoas ; [4] UFAL; [5] Instituto de Química e Biotecnologia / Universidade Federal de Alagoas

A quantitative high-throughput urine NMR metabolomics platform is presented with all the experimental details on.

3-[(E)-(4-hydroxyphenyl)iminomethyl]phenol and its reduced form as urease inhibitors: Synthesis, anti-urease activities and molecular modeling studies

https://proceedings.science/p/119465

Breno Germano de Freitas Oliveira [1]; Caroline Dohanik da Silva [1]; Edjan C.D da Silva [2]; Camila P. Pereira [1]; Luzia Valentina Modolo [1]; Ângelo de Fátima [3]; Gisele Goulart [1]; Thiago Mendonça de Aquino [2]; Júlio C.S. da Silva [2]

[1] Universidade Federal de Minas Gerais; [2] Universidade Federal de Alagoas; [3] Universidade Federal de Minas Gerais

Nitrogen (N) is essential for plant survival, growth, and crop production. In agriculture, it has been recognized as the single most vital nutrient for increasing crop yields across the globe. The use of N fertilizers is essential to maintain agricultural productivity, which is essential to provide sustenance to the human population. Urea is the most worldwide nitrogen fertilizer used; however, its enzymatic hydrolysis leads to losses through ammonia volatilization causing economic and environmental problems. To prevent this loss, urease inhibitors have been used. Among the new inhibitors synthesized by our research group, the Schiff bases have excelled results. In this work two substances, a Schiff base (3B4) and its amine derivative (3B4a), were synthesized (Scheme 1) and their in vitro antiureolytic activities were also determined. Additionally, the interactions of these substances with the urease enzyme was studied by using a molecular docking approach. The 3B4 and 3B4a were prepared with 72% and 76% yields, respectively. The in vitro antiureolytic activity of 3B4 and 3B4a (22.62 ± 6.87 and 24.16 ± 9.56, respectively) showed that both substances inhibited the urease in the same level to the positive control hydroxyurea (HU) (23.45 ± 11.95). However, it is important to mention that, differently from 3B4a, the imine 3B4 is unstable in presence of water and this can restrict the use of 3B4 as additive in N fertilizer. The molecular docking studies for 3B4 and 3B4a showed that the orientation of the hydroxyl group 3-OHPh of 3B4 and 4-OHPh of 3B4a plays an important role in the biding orientation of such subtances with the 2 nickel atoms of the urease catalytic site. Furthermore, the complex urease-3B4a showed to be more stable than complex urease-3B4, in part, due to an additional hydrogen bonding interaction between His593 with amine group and two hydrogen bonds involving hydroxyl group and the residues Ala436, Arg439 and Asp633. As a conclusion, this work have disclosed substances 3B4 and 3B4a as promising urease inhibitors, particularly amine 3B4a that is as potent as 3B4 and it is stable in aqueous medium - an important requirement for potential urease with agriculture interests. Highlights ►Urea is the most used nitrogen (N) fertilizer in the world. ►Up to 70% of urea is lost due to ammonia volatilization due to the enzymatic action of urease. ►Both urease inhibitors, prepared in excellent yields, showed as potent as the positive control, hydroxyurea. ► The amine 3B4a is the most promising urease inhibitor

4-amino-5-pyrimidinecarbonitriles derivatives: synthesis, antioxidant and antimicrobial evaluation

https://proceedings.science/p/119548

Yasmine Queiroz [1]; Jhonathan Santos [1]; Juliana Morais [1]; Loraine Morete [1]; Luciana Machado Ramos [1]; Osvaldo Pinto [1]

[1] Universidade Estadual de Goiás

The pyrimidine compounds were obtained via Biginelli-Like reaction in one-pot process using an catalyst with ionic liquid. The derivatives showed moderate antibacterial action against the strains.

A NMR study of 2-((3-aminopropyl)amino)quinolin-4(1H)-one: D/H Exchanges and Supramolecular π-stacking Interactions

https://proceedings.science/p/119636

Pedro Henrique Vasconcelos Vontobel [1]; Rodrigo dos Santos Fuscaldo [1]; Francisco Paulo dos Santos [1]; Jessie Sobieski da Costa [1]

[1] Universidade Federal do Rio Grande do Sul

Quinolone derivatives are useful in diverse applications, and are available as several drugs today, like antimalarials, antibacterial, anticancer and many others. Among all quinolone derivatives, bederocine represents a novel methionyl-tRNA synthetase (MetS) inhibitor, a potent antibiotic, which bears 2-((3-aminopropyl)amino)quinolin- 4(1H)-one (**2**) as a crucial backbone. Despite the relevance of 2, a spectroscopical data is still vague. While literature report the H8 signal as a multiplet, in our 1H NMR analysis of **2**, we obtained the H8 signal as a broad singlet, which is unexpected for this kind of aromatic nuclei. Effort has been dedicaded to understand these findings.

A sustainable access to ynones through laccase/TEMPO-catalyzed metal- and halogen-free aerobic oxidation of propargylic alcohols in aqueous medium

https://proceedings.science/p/120333

Emmanuel Dias da Silva [1]; Alana Bittencourt Vieira da Silva [1]; Alcindo Aparecido dos Santos [2]; Jefferson Princival [1]

[1] Universidade Federal de Pernambuco - UFPE; [2] Universidade de São Paulo

High yield of the products; O2 as source of oxidant; Efficient and greener approach for the synthesis of ynones.

Ácido ursólico: Isolamento das folhas de Salvia officinalis e síntese de derivados híbridos para uso em bactérias causadoras de infecções orais

https://proceedings.science/p/120508

Sayonara Batista de Oliveira [1]; Janaína Versiani [2]

[1] UNIVERSIDADE FEDERAL DE PERNAMBUCO; [2] UNIVERSIDADE DE PERNAMBUCO

We isolated ursolic acid from a cheap and easily available material (Salvia officinalis);
We synthesized 4 UA derivatives via click chemistry;
We will test them against various microorganisms.

alfa-hidróxi-1,2,3-triazóis como intermediarios de fluorenos 1,2,3-triazóis: síntese e ação antileishmanial in vitro

https://proceedings.science/p/120555

Camilla Djenne Buarque Müller [1]; Talita P. Rosa [1]; Veronica D. Silva [1]

[1] Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio)

• α-hydroxy-1,2,3-triazoles (3a-h) were synthesized
• The key step was the "click chemistry" reaction
• Compounds 3f- g presented antileishmanial action in vitro.

Amino-modified Merrifield resins as efficient heterogeneous catalysts for the diazo transfer reaction to 1,3-dicarbonyl compounds

https://proceedings.science/p/119678

Mariane Fantinel [1]; Marcus Mandolei Sá [2]

[1] Universidade Federal de Santa Catarina; [2] Univeridade Federal de Santa Catarina

Amino-modified Merrifield resins were readily prepared and successfully employed as reusable basic heterogeneous catalyst for the diazo transfer reaction to 1,3-dicarbonyl compounds to give diazo compounds in high yields.

Análise metabolômica da distribuição em níveis tróficos de alcalóides pirrólicos de invertebrados marinhos do Rio de Janeiro

https://proceedings.science/p/120652

Roberto Gomes de Souza Berlinck [1]
[1] IQSC-USP

Artificial Neural Network hybridized with Genetic Algorithm in Solid State Fermentation for the production of lipase from P. roqueforti ATCC 10110

https://proceedings.science/p/119764

Luiz Henrique Sales de Menezes [1]; Lucas Lima Carneiro [2]; Polyany Cabral Oliveira [3]; Thiago Pereira das Chagas [1]; Erik Galvão Paranhos da Silva [1]; Marcelo Franco [1]; Julieta Rangel de Oliveira [1]
[1] Departamento de Ciências Exatas e Tecnológicas, Universidade Estadual de Santa Cruz - UESC, Ilhéus, Brasil; [2] Programa de Pós-Graduação em Engenharia Elétrica - Universidade Federal de Minas Gerais - Belo Horizonte, MG, Brasil; [3] Departamento de Ciências Exatas e Naturais, Universidade Estadual do Sudoeste da Bahia - UESB, Itapetinga, Brasil

First application of RNA-AG to optimize the lipase production of P. roqueforti ATCC 10110 by FES;
5.0 x 107 artificial experiments from 28 bank experiments and triple lipase production.

Asymmetric synthesis of 2,5-dissubstituded pyrrolidines through cascade reactions

https://proceedings.science/p/120181

Paulo Gabriel Massayuki Miyake Nakaya [1]; Fábio Domingues Nasário [1]; Anita Jocelyne Marsaioli [1]
[1] Unicamp

Biocatalysis is a very important tool that has been developed and used to conduct organic reactions efficiently and with less impact on the environment. The use of enzymes or cells in catalysis has shown several satisfactory results and positive attributes [1,2] such as the reduction of steps for the separation and purification of products / intermediates. Furthermore, the fact that the enzymes have chemo-, regio- and stereoselectivity makes it possible to synthesize compounds with high enantiomeric purity. With that, we propose the synthesis of pyrrolidines scaffold by a cascade reaction using transaminases (TA) [1], followed by a spontaneous intramolecular Aza-Michael Reaction (AMR). [3] 1. Ryan, J.; Šiaučiulis, M.; Gomm, A.; Maciá, B.; O'Reilly, E.; Caprio, V. J. Am. Chem. Soc., 2016, 138, 15798. 2. Costa, B. Z.; Galman, J. L.; Slabu, I.; France, S. P.; Marsaioli, A. J.; Turner, N. J. ChemCatChem, 2018, 10, 4733 3. Hutton, T. K.; Muir, K. W.; Procter, D. J. Organic Letters 2003, 5, 4811.

Biocatalysis: Asymmetric synthesis of pyrroline alkaloids

https://proceedings.science/p/120465

Katherine Leycee Romero Orejón [1]; Vinícius Oliveira Silva [1]; Anita Marsaioli [1]
[1] Universidade Estadual de Campinas

Biocatalysis by transaminases. Spontaneous cyclization reaction. Reactions using principles of green chemistry.

Bioremediation of waters contaminated with aromatic nitriles by Aspergillus niger Tiegh 8285 isolated from cocoa southern Bahia

https://proceedings.science/p/120130

Marla Rosa Marques Ferreira Ramos [1]; Mariana Perin Mituishi [1]; Luiz Henrique Sales de Menezes [2]; Sabryna Couto Araujo [1]; Marcelo Franco [1]; Julieta Rangel de Oliveira [1]

[1] Universidade Estadual de Santa Cruz; [2] Departamento de Ciências Exatas e Tecnológicas, Universidade Estadual de Santa Cruz - UESC, Ilhéus, Brasil

It is possible to use the fungus A. niger Tiegh 8285 to treat effluents and contaminated waters. The bioremediation of environments contaminated by fungi is extremely advantageous.

BrØnsted Acidic Ionic Liquid-Catalyzed Groebke-Blackburn-Bienaymé Reaction

https://proceedings.science/p/120249

Nicolas Santos dos Anjos [1]; Agáta Ishiba Chapino [1]; Gabriela Franco Domingos dos Santos [2]; Ana Rute Santos [3]; Peter Licence [3]; Luiz S. Longo Jr. [2]

[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo/Departamento de Ciências Farmacêuticas; [3] The University Of Nottingham

The Groebke-Blackburn-Bienaymé (GBB) multicomponent reaction for the synthesis of imidazo[1,2-a]pyridines can be efficiently promoted by BrØnsted acidic ionic liquids as homogenous catalysts.

C(sp2)-H bond selenylation of imidazo[1,2-a]pyridines using diselenides and trichloroisocyanuric acid: A Green Approach

https://proceedings.science/p/120540

Marcos Roberto Scheide Neto [1]; José S. S. Neto [2]; Marcelo Straesser Franco [1]; Jamal Rafique [3]; Sumbal Saba [4]; Antonio Braga [1]

[1] Universidade Federal de Santa Catarina; [2] Departamento de Química / Centro de Ciências Físicas e Matemáticas / Universidade Federal de Santa Catarina; [3] Instituto de Química / Universidade Federal de Mato Grosso do Sul; [4] Centro de Ciências Naturais e Humanas / Universidade Federal do ABC

• Atom Economy, short reaction time; Reaction performed at room temperature using green solvent; Open to the air atmosphere; Non-toxic system.

Caracterização fotofísica e efeito da adição de TFA na fluorescência de derivados de 6-amino-4-quinolona

https://proceedings.science/p/120328

Maria Cecília B. V. de Souza [1]; Amanda Costa [1]; Micaeli Moreira [2]; Rodolfo Teixeira [2]; Vanessa Oliveira [3]; Fernanda da Costa Boechat [1]; Nanci Lucas [4]; Pedro Batalha [3]

[1] Universidade Federal Fluminense; [2] UFRJ; [3] Instituto de Química / Universidade Federal Fluminense; [4] Universidade Federal do Rio de Janeiro

Fluorescent quinolone derivatives. Emission profile modulated by acid/base equilíbrium. pH dependent fluorescente sensors.

Catalisadores de nióbio em reações multicomponentes para preparação de imidazois e diidropirimidinonas

https://proceedings.science/p/120501

Pamella Moreira Monte [1]; Anna Paula Marques [1]; José Barros [1]; Tiago Silva [1]

[1] Universidade Federal do Rio de Janeiro

This project aims to employ niobium catalysts in the synthesis of imidazoles and dihydropyrimidinones. Both of these heterocycles are present in drugs and natural products.

Chemical profiling of cotton leaves by UPLC-qTOF MS and CG-MS

https://proceedings.science/p/119706

Erika Thalyta Veras Pereira [1]; Arlindo Leal Boiça Junior [2]; Carlos Alexandro de Freitas [2]; Maria Fatima das Gracas Fernandes Silva [1]; Joao Batista Fernandes [1]; Moacir Forim [1]

[1] Departamento de Química, Universidade Federal de São Carlos; [2] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Cotton is a crop of important economic value. According to CONAB, Brazil was responsible for 6% of the world production of cotton lint in the crop years 2006/07 to 2016/17, ranked fifth among world cotton producers. For this importance, studies have been carried out to improve the quality and quantity of the fiber produced and the plant's resistance against pests (QIN et al.,2017; SUN et al., 2017). The search strategies to understand the defense mechanisms used by cotton plants and the chemical mapping of as many metabolites as possible is an actual necessity. However, the metabolomic study is still a challenge, having several critical steps, such as the choice of solvent, extraction protocols and analytical method, due to the wide chemical diversity of the metabolites in the botanical matrices. As a result, a limited profile is observed, for example because of the extraction window, and not the totality of the metabolites. Thus, the use of ultra-performance liquid chromatography coupled to a quadrupoletime-of-flight mass spectrometer (UPLC-qTOF MS) and gas chromatography connected to a mass spectrometer (GC-MS Shimadzu TQ8030) techniques complement each other by increasing the field of observation of plant profiles (KIM; VERPOORTE,2009). Thus, this study proposes a methodology for the realization of a chemical profile of cotton leaves, include ten different cultivars. The screening of plant metabolites was carried out using a (UHPLC-QTOF), being the freeze dried leaf samples (0.15 g) extracted in 3 mL of methanol/H2O (8:2) by using an Ultra-Turrax (Ika T-25, Staufen,Germany). The CG-MS, samples were prepared by obtaining the leaf extract by turbolysis using 4ml MeOH/CH3Cl (1:1), being the extract dried and derivatized with BSTFA. The substances were identified by comparison with databases for both techniques. The UPLC-qTOF MS analysis resulted in 472 compounds, of which, for instance, 23 compounds have been identified. The observed metabolic variety comprises substances of the classes of polyphenols, phenols, terpene aldehydes, flavonoids, alkaloids, amino acids among others. The flavonoids hesperidin and rutin and the alkaloid resperin are, for example, some of the compounds for the first time identified in this work as cotton leaves components. In the CG-MS analysis 132 substances were observed, being some compounds already identified, such as gallic acid, linolenic acid, L-leucine, niacin, hydroxyisovaleric acid, caryophellene and sugars. The analyzes were satisfactory with the observation of several substances, once that some of them are known to be a plant defense response, and, in addition to contributing to the identification of substances not yet related to cotton. This work is an important support for understanding of the resistance mechanisms may provide new paths for sustainable cotton production with the development of resistant genotypes, or by new chemical control products.

Chemical study of the bioactive carbohydrates from Hypsizygus marmoreus (Peck) H. E. Pigelow ("white" strain)

https://proceedings.science/p/120642

Ruberney da Silva de Oliveira [1]; Maria Carolina Bezerra Di Medeiros Leal [2]; Sthefany Rodrigues Fernandes Viana [3]; Elaine Rosechrer Carbonero [1]

[1] Universidade Federal de Goiás; [2] Universidade Federal de São Carlos; [3] YUKI Cogumelo

H. marmoreus is highly valued for its medicinal properties; Polysaccharides are their main bioactive compounds; Glycogen-like -glucan, heterogalactan, and two different -glucans were isolated.

Chemoenzymatic process for synthesis of pyrrolizidine alkaloids

https://proceedings.science/p/120269

Vinícius Oliveira Silva [1]; Katherine Leycee Romero Orejón [1]; Anita Marsaioli [1]

[1] Universidade Estadual de Campinas

One-pot process. Enantioselective reductive amination catalyzed by transaminases. Process using principles of green chemistry.

Coffee βN-alkanoyl-5-hydroxytryptamides – synthesis and antinociceptive evaluation

https://proceedings.science/p/120450

Fernanda Lima [1]; Camila Martins [1]; Thais Biondino Sardella Giorno [1]; Fernando Silva [2]; Patricia Dias Fernandes [1]; Claudia Moraes de Rezende [1]

[1] Universidade Federal do Rio de Janeiro; [2] Universidade Federal Fluminense

• The synthesis of different N-acylated serotonins using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and dimethylaminopyridine (DMAP) as coupling reagents is a simple and effective route.

Controle regioquímico da adição nucleofílica a isoquinolinodionas: Síntese total da elipticina e da isocaulibugulona A

https://proceedings.science/p/120565

Bruno Serikava [1]; Paulo Cesar Muniz de Lacerda Miranda [1]; Joaquim Castro [1]

[1] Universidade Estadual de Campinas

Ellipticine was synthesized in six steps starting from the readily available 2,5-dimethoxyisoquinoline. The regioselectivity during our synthetic route happens due to an N-oxide intermediate.

Derivados N-fenil-3-carboxamida-cumarínicos como potenciais inibidores de urease

https://proceedings.science/p/120443

Marciéli Fabris [1]; Priscila Goes de Camarcgo [1]; Fernando César Macedo Júnior [1]; Marcelle de Lima Ferreira Bispo [1]

[1] Universidade Estadual de Londrina

All synthesized derivatives showed relevant %UI against jack bean urease. Some derivatives showed IC50 values comparable to the standard thiourea, indicating that they could act as urease inhibitors.

Design and synthesis of organocalcogen pillar[5]arenes as catalysts for bromination reactions of alkenes

https://proceedings.science/p/119610

Ingrid Cavalcanti Chipoline [1]; Vanessa do Nascimento [2]; Beatrice Brasil [3]

[1] Universidade Federal Fluminense; [2] Universidade Federal Fluminense - UFF; [3] Universidade Federal Fluminense -UFF

This work presents the synthesis and application of a selenium- and tellurium-pillar[5]arenes as an efficient and ecofriendly catalyst for bromination reaction.

Design and synthesis of selenium-naphthoquinone derivatives as anti-tubercular leads against clinical multidrug resistant isolates of M. tuberculosis

https://proceedings.science/p/119958

Ruan Carlos Ribeiro [1]; Daniel Boechat [1]; Matheus Gonzaga de Moraes [1]; Wellington Silva [2]; Iris Di Leo [1]; Anne Villela [3]; Bruno Abbadi [3]; Luiz Augusto Basso [3]; Luiz da Silva [2]; Marcela de Moraes [1]; Vanessa do Nascimento [4]; Vitor Ferreira [1]; Fernando de Carvalho da Silva [1]

[1] Universidade Federal Fluminense; [2] Universidade Federal do Rio de Janeiro; [3] Pontifícia Universidade Católica do Rio Grande do Sul; [4] Universidade Federal Fluminense - UFF

A series of menadione-derived selenoesters was prepared with good yields and had their activity evaluated against M. Tuberculosis H37Rv and multidrug resistant clinical isolates (CDCT-16 and CDCT-27).

Development of aryl-quinolines as potential ligands for transition metal complexes

https://proceedings.science/p/119614

Marcio Hayashi [1]; Caio Costa Oliveira [1]
[1] Universidade Estadual de Campinas

- Synthesis of quinoline derivates ligands in 4 steps.
- Suzuki coupling in last step

Divergent / Complementary Performance of Organochalcogenides as Antimicrobial Agents

https://proceedings.science/p/120358

Tay Zugman [1]; Felipe Borges [1]; Mara Dalmolin [1]; Pamela Bandeira [1]; Debora Scariot [2]; Francielle Garcia [2]; Alfredo Oliveira [1]; Celso Vataru Nakamura [2]; Leandro Piovan [1]
[1] Departamento de Química / UFPR / Universidade Federal do Paraná; [2] Centro de Ciências da Saúde / UEM / Universidade Estadual de Maringá

Antimicrobial assays of selenium- and tellurium-containing ketones and amines disclosed organoselenides as preferential antifungal agents while organotellurides perform better as antibacterial agents.

Efficient Eco-Friendly Solvent-Free Alkenes Aminoselenation

https://proceedings.science/p/119733

Luana da Silva Gomes [1]; José S. S. Neto [2]; Iris Di Leo [1]; Claudio Santi [3]; Vanessa do Nascimento [4]
[1] Universidade Federal Fluminense; [2] Universidade Federal de Santa Catarina; [3] University of Perugia; [4] Universidade Federal Fluminense - UFF

In this work a new eco-friendly approach to the seleno-functionalization of alkenes through a fast, solvente- and metal- free method was developed.

Electricity and Catalysis: A Powerful Combination toward the Synthesis of Vicinal Diazides and Diamines

https://proceedings.science/p/120302

Luiz Fernando Toneto Novaes [1]; Jinjian Liu [2]; Niankai Fu [2]; Song Lin [2]
[1] Department of Chemistry and Chemical Biology / Cornell University; [2] Cornell University

An electrochemical diazidation of alkenes using only 0.5 mol% of catalyst is reported in this abstract. Use of chiral Mn-porphyrins led to formation of vicinal diazides in enantioselective fashion.

Electro-polymerization and spectroelectrochemical properties of a new 2,5-di(thienyl)pyrrole bearing Fluorene-9-Carboxilyc acid.

https://proceedings.science/p/119621

Dimas José da Paz Lima [1]; Jorge de Lima Neto [1]; Adriana Santos Ribeiro [1]; Luis Paulo Alves da Silva [1]
[1] UFAL

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Electrochemical study of naphthoquinone-based hydrazone hybrids: a promising proposal for the development of new drugs.

https://proceedings.science/p/120226

Thaissa Lúcio Silva [1]; Danyelle Cândido Santos [1]; Cleônia Roberta Melo Araújo [2]; Marília Oliveira Fonseca Goulart [3]
[1] Universidade Federal de Alagoas - Campus de Arapiraca/Núcleo de Ciências Exatas (NCEx) – Arapiraca-AL; [2] Universidade Federal do Vale do São Francisco/Colegiado de Ciências Farmacêuticas; [3] Universidade Federal de Alagoas/Instituto de Química e Biotecnologia

We investigated the electrochemical behavior of naphthoquinone-based hydrazone hybrids, strong candidates as prototypes of new, more potent, and selective antineoplastic drugs.

Enantioselective Aza-Wacker-type reaction promoted by Pd(II) and oxazolines or imidazolines ligands as catalytic system

https://proceedings.science/p/120094

Elaine Miho Ariga [1]; Bianca Yumi Ohira [1]; Ariadne de Jesus Vicente [1]; Elisângela Vinhato [1]; Alessandro Rodrigues [1]
[1] Universidade Federal de São Paulo

Enantioselective Aza-Wacker type reaction of allylic carbamates. Catalytic system formed by Pd(II) and chiral ligands such as oxazolines and imidazolines.

Enantioselective Bromoaminocyclization Reactions via Organocatalysis

https://proceedings.science/p/119765

Jullyane Emi Matsushima [1]; Francisco Ribeiro [2]; Thiago Correra [2]; Alessandro Rodrigues [1]
[1] Universidade Federal de São Paulo; [2] Universidade de São Paulo

Development of a new methodology of enantioselective bromoaminocyclization of carbamates by organocatalysts. Regio-/stereoselective control in bromoaminocyclization reactions of allyl tosylcarbamates.

Enantioselective Heck Arylations of Endocyclic Enelactams Using N,N Ligands

https://proceedings.science/p/119566

Ingredy Bastos Braga [1]; Emilio Carlos de Lucca Junior [1]; Ricardo Almir Angnes [2]; Ataualpa Braga [2]; Carlos Roque D. Correia [1]
[1] Universidade Estadual de Campinas; [2] Universidade de São Paulo

In this work, we developed a new method for the enantioselective arylation of endocyclic enelactams via Heck reactions. The Heck products can be obtained in good yields and enantiomeric excesses up to 90%. The reaction mechanism was also investigated via DFT in silico studies.

Enantioselective Total Synthesis of (S)-nuciferine

https://proceedings.science/p/120471

Tamiris Reissa Cipriano da Silva [1]; Cristiano Raminelli [1]
[1] Universidade Federal de São Paulo

Benzyne chemistry and enantioselective hydrogenation were employed in the total synthesis of (S)-nuciferine, which presents potential affinity for the serotonin 5-HT2A receptor.

Enzymatic Kinetic Resolution of Secondary Alcohols under continuous flow conditions

https://proceedings.science/p/120169

Bárbara Maia de Viveiros [1]; Mauro Gomez [2]; Raquel Ana Apela Leão [2]; Rodrigo Octávio Mendonça Alves de Souza [2]
[1] Universidade Federal do Rio de Janeiro; [2] Grupo de Biocatálise e Síntese Orgânica, Instituto de Química, Universidade Federal do Rio de Janeiro, RJ

Enzymatic kinetic resolution of alcohols. Active pharmaceutical ingredients synthesis. Use of lipase Candida antactica B for chiral center resolution.

Estudo da Estabilidade Oxidativa pelo Método Rancimat do Biodiesel Aditivado com Aminas Aromáticas

https://proceedings.science/p/119527

Gabrielly dos Santos Maciel [1]; Philipe Diego Araújo da Silva [1]; Antonia Lucia de Souza [1]; Neide Queiroz [1]
[1] UFPB

Highlights Study of Oxidative Stability by the Rancimat Method of Biodiesel Added with Aromatic Amines. Induction period values showed protective effect of aromatic amines against oxidative biodiesel. Extent of protection factor in the samples was dependent of aromatic amines as antioxidant. Resumo/Abstract Dada a importância do biodiesel para o Brasil e para o mundo, inúmeras pesquisas vêm sendo desenvolvidas para garantir que este seja um combustível de qualidade à altura das tecnologias empregadas no desenvolvimento dos motores a diesel. A susceptibilidade do biodiesel à degradação oxidativa compromete sua qualidade durante armazenamento e transporte, ocasionando assim dificuldades na manutenção da integridade do biocombustível vendido ao consumidor final. Uma tendência seguida pela indústria de biodiesel tem sido o uso de aditivos antioxidantes, onde comumente se utiliza compostos fenólicos tais como o terc-butilhidroquinona (TBHQ), butil-hidroxitolueno (BHT), e butil-hidroxi-anisol (BHA). Entretanto aminas aromáticas também demonstram eficiência no retardo da degradação oxidativa de combustíveis (Rashed et al., 2016; Joshi et al., 2013). Diante desta problemática, o presente trabalho avaliou a estabilidade oxidativa de amostras de biodiesel aditivadas com antioxidantes aminados, a saber, 3,4-diaminotolueno (DAT), difenilamina (DIF), N-fenil-o-fenilenodiamina (DNO) e N-fenil-p-fenilenodiamina (DNP), na concentração de 5,00 mmol.kg-1. Todos os parâmetros físico-químicos estudados para as amostras de biodiesel estavam dentro dos limites estabelecidos pela regulamentação vigente. Os valores de período de indução (PI) das amostras de biodiesel sem e com aditivo (DAT, DNO, DNP e DIF) obtidos por meio do método Rancimat são mostrados na Tabela. As amostras BMA (biodiesel metílico do óleo de algodão) e BMRR (biodiesel metílico do óleo residual residencial), as quais são constituídas principalmente de ésteres graxos insaturados, não alcançaram o limite de 8 h estabelecido pela ANP. No entanto, após adição de DAT, DNP e DNO houve aumento do PI acima do exigido, exceto para amostra BMRR/DNP. Antioxidante 5 mmol.kg-1 PI (h) das amostras de biodiesel BMA BMRR BMRC Sem 5,78 ± 0,30 6,47 ± 0,19 11,64 ± 0,54 DAT 10,07 ± 0,09 9,51 ± 0,07 21,86 ± 0,06 DNO 13,33 ± 0,22 9,45 ± 0,07 21,62 ± 0,22 DNP 9,76 ± 0,07 6,97 ± 0,43 22,65 ± 0,33 DIF 5,69 ± 0,46 4,86 ± 0,11 11,18 ± 0,12 Diferentemente, a amostra de BMRC (biodiesel metílico do óleo residual comercial), composta principalmente de oleato de metila e hexadecanoato de metila, apresentou valor de PI acima de 8 h. Entretanto, estabilidade oxidativa adicional pode ser alcançada com a adição de DAT, DNO e DNP. Ao contrário do aditivo DIF que não mostrou efeito protetivo, evento também observado nas amostras de BMA e BMRR com este aditivo. O efeito protetor de 130 % obtido para a amostra BMA aditivada com DNO (921 ppm) foi maior do que o observado por Saluja et al. (2016), evidenciando a eficiência deste antioxidante frente ao BHT (88%) e BHA (94%) na concentração de 1000 ppm e próxima ao TBHQ (170%) relatado por Avinash et al. (2018). Foi possível verificar que as amostras de BMRR com os antioxidantes DAT (9,51 h) e DNO (9,45 h) apresentaram PI um pouco maior ao relatado para amostras contendo BHA e BHT (9,1 h), estudadas por Saluja et al. (2016). Assim como a composição do biodiesel, as diferenças de estabilidade oxidativa observadas entre as amostras podem ser explicadas pelas estruturas químicas dos antioxidantes. Para concluir, tem-se que as aminas aromáticas são promissoras no controle da estabilidade oxidativa do biodiesel. Avinash, A.; Sasikumar, P.; Murugesan, A. Renew. Energy 2018, 127,1-33. Joshi,G.; Lambar, B.Y.; Rawat, D.S.; et al. Ind. Eng. Chem. Res. 2013, 52, 22. Rashed, M.M.; Masjuki, H.H.; KALAM, M.A.; et al. RSC Advances 2016, 27, 22436-22446. Saluja, R.K.; Kumar, V.; Sham, R.; Renew. Sust. Energ. Rev. 2016, 62, 166-181. Agradecimentos/Acknowledgments À UFPB, Capes, CNPq e NPE_LACOM.

Estudo reacional para a obtenção de imidazóis a partir de isatinas

https://proceedings.science/p/120291

Jan Pierre de Paiva Soares [1]; Gabriel Freitas do Rio [2]; Aurelio Baird Buarque Ferreira [1]
[1] Universidade Federal Rural do Rio de Janeiro; [2] UFRRJ

Reaction study for obtaing imidazoles from isatins. This work aims to obtain an effective, low cost and easily reproducible method for the synthesis of imidazoles from isatins.

Estudo termodinâmico em meio de membrana mimética aniônica de peptídeos modificados de Fenilseptina

https://proceedings.science/p/120184

Flaviane Cristina Oliveira [1]; Amanda Souza Félix [1]; Carolina Silva Ferreira [1]; Victor Hugo Oliveira Munhoz [1]; Rodrigo Moreira Verly [1]
[1] Universidade Federal dos Vales do Jequitinhonha e Mucuri

Influence of The position of The D amino acid residue on The activity of synthetic peptides, compared to peptides of origin.

Explorando a Reatividade de Aldeídos na Reação de Groebke-Blackburn-Bienaymé Catalisada por Líquidos Iônicos Ácidos de Bronsted

https://proceedings.science/p/120436

Nicolas Santos dos Anjos [1]; Agáta Ishiba Chapino [1]; Naara Santos [1]; Luiz S. Longo Jr. [2]
[1] Universidade Federal de São Paulo; [2] Universidade Federal de São Paulo/Departamento de Ciências Farmacêuticas

A series of nine imidazo[1,2-a]pyridines can be efficiently obtained in good to excellent yields via Groebke-Blackburn-Bienaymé (GBB) reaction catalyzed by the BrØnsted acidic ionic liquids.

Extraction of essential oil of oregano (Origanum vulgare) by Italian coffee maker: a new trick to an old undergraduate experiment

https://proceedings.science/p/119774

Bruna Costa Cerqueira [1]; Amanda Rosa Alves; Edson E. Silva [1]; SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

Origanum vulgare, Steam distillation, Italian coffee maker, essential oil.

Extraction of paracetamol: chemical comparison between reference and generic medicines as an undergraduate experiment

https://proceedings.science/p/119949

Lourenço Santana [1]; Orlando Barboza [1]; Fernando Alves Barretto [2]; Wilson Lopes [2]; SILVIO CUNHA [2]
[1] Universidade do Estado da Bahia; [2] Universidade Federal da Bahia

Medicines are employed in undergraduate courses as motivational strategy, and the development of new experiments performable in simple laboratory infrastructure deserve attention. The experiment herein developed compares the extraction of paracetamol from reference and generic drugs. Paracetamol was chosen due to its general use by the population and ease access. Tablets were used from two commercial sources of reference (750 mg) and generic drugs (750 and 500 mg) purchased from local drugstores. For the average weight analysis 20 tablets were individually weighed by each group. Two tablets were pulverized and extracted in triplicate with ethyl acetate. After filtration and solvent evaporation, the active ingredient was obtained and identified by melting point and FTIR

analyzes. The experiment was carried out by different groups of students and at different times, There was similar performance between the extractions of each group, which corroborates the analysis of pharmaceutical equivalence. Comparing different groups of students at different times, there was change in the mass of paracetamol extracted, which may be associated with changes in the excipient content of drugs over time. The procedure was efficient since there was similarity between the results obtained for generic and reference drugs. Therefore, it is consistent for use in the undergraduate classroom because allows discussion on pharmaceutical equivalence and interchangeability, involves simple laboratory infrastructure, execution and materials are easily obtained.

Funcionalização dirigida de arenos e heteroarenos visando a síntese de substâncias de interesse medicinal

https://proceedings.science/p/120650

Giuliano Cesar Clososki [1]
[1] USP

Graphene oxide copper catalysts for azide–alkyne 1,3- cycloaddition

https://proceedings.science/p/119445

Ronaldo Oliveira [1]; Cecilãne Regina Dioclecia da Silva [1]; Kethully Lima [2]; Thaises Lima [2]; Patrícia Araújo [2]; Elmo Araújo [2]
[1] Universidade Federal Rural de Pernambuco; [2] Universidade Federal de Pernambuco - UFPE

Graphene oxide composite functionalized with copper acetate and reduced graphene oxide functionalized with copper oxide were prepared and used to promote azide-alkyne 1,3dipolar cycloaddition reaction

Hydroquinolinone synthesis by reaction of 2,5-diamino-1,4-benzoquinone with 5-arylidene derivatives of Meldrum's acid

https://proceedings.science/p/120127

Edson E. Silva [1]; SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

Hydroquinolinones were synthesized through reaction of 2,5-diamino-1,4-benzoquinone and 5-arylidene derivatives of Meldrum's acid under microwave heating.

Identificação das classes de metabólitos secundários e isolamento de Kaempferitrin das folhas de Clitoria guianensis.

https://proceedings.science/p/119861

Állefe Barbosa Cruz [1]; Camila Luiza Cunha [2]; Daniela Franscisca Soares [3]; Juliana Cristina Holzbach [4]
[1] Universidade Federal do Tocantins ; [2] Universidade Estadual Paulista; [3] Universidade Federal do Tocantins; [4] Universidade Federal do Tocantins

Highlights Phytochemical study of C. guianensis. Identification of classes of secondary metabolites. Nuclear Magnetic Resonance for substance identified.

Influence of the solvent on the preparation of DB18C4 crown ether

https://proceedings.science/p/119742

Rodolpho Alessandro Nesta Silva [1]; Sergio A Marques de Lima [2]; Marian Rosaly Davolos [1]; Ana Maria Pires [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"; [2] Universidade Estadual Paulista-Unesp

The synthesis through two distinct routes of the crown ether Dibenzo-18-crown-4 was investigated and the best one leaded with success into a compound with higher yield and purity degree.

Isolamento de fungos celulolíticos de solo do ambiente amazônico e sua aplicação na produção de celulases

https://proceedings.science/p/119977

Taiana Sousa Bezerra [1]; Darlisson de Alexandria Santos [2]
[1] UNIFESSPA - UNIVERSIDADE FEDERAL DO SUL E SUDESTE DO PARÁ.; [2] Universidade Federal do Sul e Sudeste do Pará

A celulose é o recurso renovável mais abundante para uso como substrato na produção de combustíveis e produtos químicos alternativos1. Muitos esforços foram feitos para realizar a hidrólise da celulose, a fim de utilizar os açúcares liberados para a produção de bioetanol. Nesse contexto, foi introduzido o uso de microrganismos para produzir enzimas que realizam essa reação2. Neste estudo, foi realizado isolamento e bioprospecção de fungos do solo de ambiente amazônico capazes de produzir enzimas lignocelulolíticas visando a produção de celulases. Os fungos foram cultivados sob fermentação em estado sólido em frascos Erlenmeyer (125 mL) que continham farelo de trigo (5,0 g) e 10 mL da solução de Mendel. O inóculo foi feito com solução de esporos para a padronização entre todas as linhagens, na concentração de 5.105 esporos/grama de substrato e incubados em estufa por 3 dias a 32 °C. Após o período de crescimento foi realizada a extração das enzimas totais. A solução da enzima bruta foi obtida adicionando 50 mL de tampão acetato de sódio (0,5 M, pH 4,5) ao meio de cultivo. Em seguida o meio foi macerado e triturado e a solução foi agitada vigorosamente durante 60 min. A mistura foi filtrada a vácuo para a retirada da fração sólida. A solução resultante foi usada posteriormente para avaliação da atividade celulolítica do extrato enzimático. No teste de atividade foi utilizada uma tira de papel de filtro (6 cm x 1 cm), que foi enrolada em formato espiral e colocada dentro do tubo de ensaio. Em seguida, adicionou-se 2 mL de tampão citrato (pH 4,8, 50 mM) e 1 mL do extrato enzimático. Os tubos foram então mantidos a 50 °C por 60 min para que ocorresse a reação. A quantidade de açúcares redutores produzida a partir da hidrólise da celulose do papel de filtro foi medida pelo método DNS. Foram oito as linhagens fúngicas isoladas e estudadas quanto à sua atividade celulolítica, sendo atribuído às mesmas, códigos de identificação. Das oito linhagens isoladas e purificadas, cinco delas foram avaliadas acerca de sua capacidade em produzir enzimas celulases. Observou-se que as linhagens fúngicas estudadas apresentaram valores de atividade que denotam que as mesmas possuem um bom potencial de estudo para a produção de celulases. Dentre as linhagens, podemos destacar A1C2-03, A1C2-05 e A1C2-06, que apresentaram atividades celulolíticas semelhantes e bem promissoras para a continuação da pesquisa, sobretudo na realização de experimentos para determinar as melhores condições de cultivo e reacionais para a obtenção de uma maior atividade. A linhagem A1C2-03 já foi estudada quanto ao melhor período de cultivo em meio sólido contendo farelo de trigo. O cultivo foi realizado por 10 dias, sendo feita a determinação da atividade celulolítica após cada período de 24 h. Observou-se, então, que o melhor dia de crescimento para esta linhagem é no 3º dia após seu inoculo, apresentando uma atividade enzimática celulolítica de 0,5 U.g-1. As próximas etapas deste trabalho envolvem o estudo de outras variáveis de cultivo (pH, temperatura, teor de umidade), o estudo das melhores condições reacionais para as enzimas produzidas por esta linhagem bem como realizar os mesmos experimentos para as linhagens A1C2-05 e A1C2-06. Referências: 1-Mohammadi, et al. Renewable and Sustainable Energy Reviews, v. 15, p. 4255-4273, 2011. 2-Souza, et al. Biocatalysis and Agricultural Biotechnology, v. 14, p. 183-188, 2018

Late-Stage Oxidation of C-H Bonds in ent-Kaurene Diterpenoids

https://proceedings.science/p/120246

Laiéli dos Santos Munaretto [1]; Ana Carolina Ferreira Soares Rocha [2]; Vladimir Constantino Gomes Heleno [2]; Emilio Carlos de Lucca Júnior [1]
[1] Universidade Estadual de Campinas; [2] Universidade de Franca

Methodologies that directly functionalized C(sp3)—H bonds of complex molecules are significant because of their potential to deliver new compounds with high biological potential. Here we report late-stage oxidation strategies of kaurenoic acid.

Mecanoquímica e síntese orgânica: de polímeros a policíclos e lausona
https://proceedings.science/p/120653

SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

Mechanochemical diastereoselective synthesis of 3-acyl-thioenaminones.
https://proceedings.science/p/119921

Talita Santana Nascimento [1]; Iva Souza de Jesus [1]; SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

A new method for the synthesis of 3-acyl-thioenaminones was developed through reaction between enaminones and phenyl isothiocyanate under mechanochemical condition.

Metal-Free Photoarylation of Diazines with Aryldiazonium Salts
https://proceedings.science/p/120405

Rodrigo Costa e Silva [1]; Lucas Facuri Villela [1]; Timothy Brocksom [1]; Kleber Thiago de Oliveira [1]
[1] Universidade Federal de São Carlos

The photoarylation of diazines with aryldiazonium salts in dimethylsulfoxide is described, using blue LED light.

Metal-Free Photoinduced Hydroalkylation Cascade Protocol Enabled by Electron-Donor-Acceptor Complex
https://proceedings.science/p/119421

Pablo Silva Carneiro [1]; José Tiago Correia [1]; Gustavo Piva [1]; Camila Kisukuri [2]; Elias André [1]; Bruno Pires [2]; Márcio Weber Paixão [1]
[1] Departamento de Química / Universidade Federal de São Carlos; [2] Universidade Federal de São Carlos
Photoinduced SET process enable by Electron-Donor-Acceptor (EDA) complex. Photocatalysis under continuous-flow conditions. Applicability of the protocols to commercially available drugs.

Microwave-assisted multicomponent synthesis of julolidines using silica-supported calix[4]arene as heterogeneous catalyst
https://proceedings.science/p/119427

Walysson Ferreira de Paiva [1]; Ingredy Bastos Braga [2]; João Vitor de Assis [1]; Sandra Milena Bonilla Castañeda [1]; Ángel Gabriel Sathicq [3]; Valeria Palermo [3]; Gustavo Pablo Romanelli [3]; Ricardo Natalino [1]; Marcio José da Silva [1]; Felipe Martins [4]; Gustavo Senra Gonçalves de Carvalho [5]; Giovanni Amarante [5]; Sergio Antonio Fernandes [1]
[1] Universidade Federal de Viçosa; [2] Universidade Estadual de Campinas; [3] Universidad Nacional de La Plata; [4] Universidade Federal de Goiás; [5] Universidade Federal de Juiz de Fora
In this work, the multicomponent Povarov reaction was used for the synthesis of tetrahydrofuranjulolidines catalyzed by Si(*n*)CX[4]SO3H and assisted by microwave. The heterogeneous catalyst was synthesized from the *p*-sulfonic acid calix[4]arene by the sol-gel technique. The Povarov reaction is a multicomponent reaction between an aniline, an aldehyde and an alkene or alkyne, catalyzed by Lewis or Brønsted acids, and can provide tetrahydroquinolines, quinolines or julolidines as products, depending on the reactive conditions employed. In this work, 24 julolidines were synthesized from different *p*-substituted anilines, formaldehyde and 2,3-dihydrofuran. The optimized conditions for the synthesis were: aniline (0.5 mmol), formaldehyde (1.5 mmol), 2,3-dihydrofuran (1.5 mmol), temperature of 150 °C, reaction time of 10 minutes, catalyst concentration of 0.5 mol%, in the absence of solvents. Yields ranged from 58 to 97%. The julolidines were obtained as a mixture of diastereoisomers, which were separated by a silica gel chromatography column, providing 12 julolidines with *cis* stereochemistry and 12 julolidines with (±)-*trans*

stereochemistry. Compounds were identified and characterized by mass spectrometry, infrared spectroscopy, chiral column HPLC and 1H and 13C Nuclear Magnetic Resonance. The great advantage of the developed methodology is the short reaction time, the operational simplicity and the absence of solvents, factors that help to reduce the formation of residues and go according to the principles of green chemistry.

Molecular hybridization as strategy in chromene-dihydropyrimidinones and xanthene-dihydropyrimidinones synthesis.

https://proceedings.science/p/120543

Samuel Santos [1]; Luiz Antonio Mazzini Fontoura [2]; Dennis Russowsky [1]
[1] Universidade Federal do Rio Grande do Sul; [2] Universidade Luterana do Brasil

Xanthene-DHPMs and Chromene-DHPMs hybrid compounds were synthesized by the CuAAC method as potential multifunctional compounds.

N,1-Diphenyl-1H-tetrazol-5-amine: a new green synthesis and reactions with trihaloisocyanuric acids

https://proceedings.science/p/119904

Adriana Marques Moraes [1]; Tiago Lima da Silva [2]; Marcio de Mattos [3]
[1] Universidade Federal do Rio de Janeiro (UFRJ); [2] UFRJ; [3] Instituto de Química / UFRJ

5-Aminotetrazoles are important heterocyclic compounds that can be prepared by reaction of thioureas with toxic HgCl2 followed by treatment with NaN3 in basic media.1 We have developed a new, green and simple methodology for the preparation of N,1-diphenyl-1H-tetrazol-5-amine by reaction of N,N'-diphenylthiourea with trichloroisocyanuric acid (0.16 mmol), sodium azide (0.55 mmol) and triethylamine in different solvents (7 mL). Using EtOAc our methodology gave a superior yield (80 %) than the previously reported with toxic HgCl2 (70 %).1 Further reaction of N,1-diphenyl-1H-tetrazol-5-amine with trihaloisocyanuric acids produced the corresponding halogenated derivatives of the 5-aminotetrazole in high regioselectivity, being the iodinated product an unpublished one. The halogenated derivatives are solid and were purified by recrystallization. In the purification process there was a significant loss of the products which caused low yield (30-50%), however it is important to highlight this purification succeeded to provide the para selectivity of the halogenated compounds and further studies will be done to promote less loss of materials.

New Thiopyrimidinones from Base-catalyzed Thiol-Ene Coupling as Aldose Reductase Inhibitors

https://proceedings.science/p/120516

Sidney Gustavo Diniz Feitosa [1]; Janaína Versiani dos Anjos [2]
[1] UNIVERSIDADE FEDERAL DE PERNAMBUCO; [2] UNIVERSIDADE DE PERNAMBUCO

Unprecedented modification of 2-thiopyrimidinones via thiol-ene coupling; We synthesized 35 2-thiopyrimidinones derivatives; Some derivatives showed good aldose reductase inhibition.

Organocatalisadores derivados da Cinchona: Síntese e Aplicação em Reações de Michael Estereosseletiva envolvendo nitrociano-compostos

https://proceedings.science/p/119649

Priscila Machado Arruda Soares [1]; Elisângela Vinhato [1]; Alessandro Rodrigues [1]
[1] Universidade Federal de São Paulo

Synthesis of bifunctional organocatalysts from Cinchona alkaloid-derived.
Evaluation of organocatalysts in the stereoselective Michael Reaction for the synthesis of multifunctionalized compounds.

Otimização da síntese de 5-amino-N,1-difenil-1H-tetrazol a partir de difeniltioureia

https://proceedings.science/p/120574

Isabela Graciano [1]; Paula Fernandes de Aguiar [1]; Tiago Silva [1]
[1] Universidade Federal do Rio de Janeiro

This work aims to improve the usual syntheses of tetrazoles from thioureas, introducing less toxic reagents and a more effective way of heating, considerably reducing the reaction time.

Oxidation of azaindoles

https://proceedings.science/p/119665

Cintia Maria Carneiro Franco Lima [1]; Mauricio Victor [1]; Till Opatz [2]
[1] UFBA; [2] JGU

Azaindoles may be used as intermediates in the preparation of some biologically active substances.1 They are bioisosteres of an indole moiety varying the position of the nitrogen atom on the benzene core: 4-,5-, 6- and 7-azaindoles.2 Three different synthetic procedures were used to perform the oxidation of 4-azaindol, 5-azaindol, 6-azaindol, 7-azaindol and the indol. The first one3 (a) was carried out by adding bromine into a mixture of 1:1 tBuOH/H2O; the second4 (b) using pyridinium bromide perbromide (PBPB) in a solution of tBuOH; and the last5 (c) synthetic methodology utilized pyridinium chlorochromate (PCC)−SiO2 as oxidizing agent. The results are shown in thefollowing Table 1. It should be noted that no oxidation was found at the entrances 8 and 9. All products were characterized by 1H and 13C NMR spectroscopy. Nine azaindoles derivatives were synthesized employing three different synthetic methodologies.

Photocatalyzed Hydrotrifluoromethylation of Dicarbonyl Compounds in Batch and under Continuous Flow Conditions

https://proceedings.science/p/120298

Gabriel Martins Ferreira Batista [1]; Pedro Pôssa de Castro [1]; Hélio F. Dos Santos [1]; Kleber Thiago de Oliveira [2]; Giovanni Amarante [1]
[1] Universidade Federal de Juiz de Fora; [2] Universidade Federal de São Carlos

Planejamento e Síntese de Derivados Pirazolil Benzenossulfonamídicos com Potencial Atividade Antibacteriana

https://proceedings.science/p/120527

Thaisa Ribeiro Henriques Quinteiro [1]; Vinicius Campos [1]; Alice Maria Rolim Bernardino [1]
[1] Universidade Federal Fluminense

This work describes the synthesis of 8 pyrazolyl benzenesulfonamide derivatives designed as potential antibacterial activity against bacterial strains of Gram-negative and Gram-positive.

Polyurethane membrane from polycaprolactone triol, 1,6-hexamethylene diisocyanate and ibuprofen®.

https://proceedings.science/p/119911

Igor Fagundes Valezan [1]; Ana Carolina Aguiar [1]; Rachel Faverzani Magnago [2]; Luiz Alberto Kanis [3]
[1] UNISUL - Universidade do Sul de Santa Catarina; [2] Universidade do Sul de Santa Catarina (UNISUL); [3] Airela Pharmacêutica

A administração de fármacos de maneira controlada vem ganhando cada vez mais espaço devido a grande objetividade e eficiência. A partir disto fez-se a síntese de uma matriz polimérica utilizando policaprolactona-triol e 1,6-hexametileno diisocianato e também com Ibuprofeno incorporado. A caracterização foi realizada com , termogravimetria, intumescimento e resistência mecânica. Com essas análises foi possível verificar que tanto a matriz

pura e com Ibuprofeno não apresentaram alterações quando submetidas a temperatura e pressão elevadas, além disso também se observou que houve dois pontos de decaimento na termogravimetria, um ponto indicando a degradação do fármaco e outro a do PU. Diante disso há evidência de que possivelmente houve a incorporação do Ibuprofeno e que o mesmo foi liberado em solução fisiológica após intumescimento.

Preparação enzimática de amidas graxas de interesse biológico derivadas de oleaginosas da Amazônia

https://proceedings.science/p/120651

Irlon Maciel Ferreira [1]
[1] UNIFAP

Production of 2-phenylethanol by biotransformation of 2-phenylnitroethane using different fungi strains

https://proceedings.science/p/119707

Darlisson de Alexandria Santos [1]; Franco Almeida [1]; Ruberney da Silva de Oliveira [2]; Sebastião Silva [1]; Marilene Nunes Oliveira [1]
[1] Universidade Federal do Sul e Sudeste do Pará; [2] Universidade Federal de Goiás

2-Phenylethanol is a well know alcohol that is characterized by its rose-like odor, being used as component in fragrance, cosmetic, and food industries1. It occurs widely in nature, mainly in essential oils extracted from rose, jasmine, carnation, and hyacinths2. However, their low concentration makes the recovery complex and expensive1,2. 2-Phenylethanol was also described as showing antimicrobial and antityrosinase activities, which aggregates more attention to its production3. 2-Phenylnitroethane, used in this work as substrate for 2-phenylethanol, is the main component of *Aniba canelilla* essential oil, corresponding to approximately 80% of the total amount. Then, it was used as substrate without any previous purification. To produce 2-phenylethanol through biotransformation of 2-phenylnitroethane, four different fungi were applied: *Aspergillus flavus* and *Rigidoporus lineatus* (isolated from copper mining residue from Mina do Sossego, Canaã dos Carajás, Pará, Brazil), *Lasiodiplodia caatinguensis* (phytopathogenic fungus from *Citrus sinensis*), and *Colletotrichum* sp. (phytopathogenic fungus from *Euterpe oleracea*). The fungi were cultivated in Erlenmeyer flasks (250 mL) containing 100 mL of malt extract solution (2%) for seven days under orbital agitation (132 rpm) at 30 ºC. Then, 50 mg of *A. canelilla* essential oil were diluted in 100 µL of dimethylsulfoxide (DMSO) and added to each fungi cultivation. Each experiment had its control by fungi cultivation without the essential oil addition. Every day (1 - 7 days), aliquots (2 mL) were removed from each experiment and extracted using ethyl acetate (2 mL) and analyzed by GC-MS in order to determine the percentage of 2-phenylnitroethane biotransformation in 2-phenylethanol. After 7 days, it was observed that the two fungi (*A. flavus*, and *L. caatinguensis*) performed the complete biotransformation of 2-phenylnitroethane in 2-phenylethanol, with special attention to *L. caatinguensis* that achieved the complete biotransformation after two days of reaction. The other two fungi (*R. lineatus*, and *Colletotrichum* sp.) partially performed the biotransformation, but *Colletotrichum* sp. also produced a not-identified compound, which will the object of future studies. Therefore, it was possible to assign that *A. flavus* and *L. caatinguensis* fungi are very promisors in 2-phenylethanol production using 2-phenylnitroethane as substrate and can be the object of study in the next steps of this work, that includes the improvement of the reactional conditions and the production of 2-phenylethanol using other substrates such as hydrolyzed lignin and cinnamyl alcohol.

Reações aldólicas assimétricas mediadas por aminocatalisadores em meio livre de solvente

https://proceedings.science/p/120545

Rafaela de Souza Martins [1]; Mathias Prado Pereira [1]; Pedro Pôssa de Castro [1]; Fernanda Irene Bombonato [1]
[1] Universidade Federal de Juiz de Fora

The preparation of novel organocatalysts for the solvent-free asymmetric aldol reaction allowed the attainment of Aldol products in up to 95% yield, 1:19 syn/anti and 98% e.e.

Reaction of Methoxybenzyl Alcohols with Trichloroisocyanuric Acid (TCCA): Ipso Substitution

https://proceedings.science/p/119486

Carlos Vinícius Pinto dos Santos [1]; Marcio de Mattos [1]
[1] Instituto de Química / UFRJ

O uso de ácido tricloroisocianúrico (TCCA) para oxidação de álcoois benzílicos tem sido um ponto de interesse recente em nosso grupo e nesse trabalho são apresentados os resultados das reacões de álcoois metóxi-benzílicos com TCCA. Foram estudados o efeito do oxidante na reação, os substituintes do anel aromático e suas posições relativas ao grupo hidróxi-metil. Em geral, os álcoois benzílicos com grupos doadores de elétrons levam à cloração eletrofílica do substrato na posição ipso: o álcool 4-metoxibenzílico forma 4-cloroanisol (98%), o álcool 4-hidroxibenzílico forma 4-clorofenol (33%) e o álcool mesitílico forma o cloro-mesitileno (31%). Por outro lado, álcoois benzílicos polimetoxilados levaram a misturas de produtos de substituição ipso do grupo hidróximetil e, predominantemente, produtos de cloração eletrofílica tradicional. Os resultados podem ser explicados através de complexo-π entre o TCCA e o substrato, onde a maior capacidade de fornecer elétrons para a redução do TCCA define o caminho reacional.

Regioselective Sythesis of Pyrazolyl-pyrimidine Hybrids of Pharmacological Interest

https://proceedings.science/p/119756

Adriano Felin Camargo [1]; Mário André Marangoni [1]; Paulo Alexandre de Moraes [1]
[1] UFSM

The regioselective synthesis of twenty novel [3-substituted 5-hydroxy-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-1-yl][6-aryl-(2-methylthio)pyrimidin-4-yl]methanones from the cyclocondensation reactions of new 6-aryl-2-(methylthio)pyrimidine-4-carbohydrazides with 4-substituted 1,1,1-trifluorobut-3-en-2-ones is reported. Human acetylcholinesterase (HsAChE) and butyrylcholinesterase (HsBChE) inhibition tests were performed on selected products in order to explore the possible pharmacological applications of these compounds. Two compounds showed significant and selective inhibitory activity for BChE.

Resolução Cinética Dinâmica de aminas primárias mediada por paládio suportado em dolomita na presença de líquidos iônicos como aditivos.

https://proceedings.science/p/120387

Matheus Boaretto [1]; Luiz Sidney Longo Júnior [1]; Fernanda Amaral de Siqueira [1]
[1] Universidade Federal de São Paulo

DKR is a methodology used to synthesize asymmetric compounds from racemic mixtures.The use of the palladium catalyst suported on dolomite together with ionic liquids provided satisfactory results.

Scandium(III) Triflate Immobilized into Polymer-Supported Ionic Liquid Phases as Catalysts for the Cyanosilylation of Aldehydes

https://proceedings.science/p/120055

Gabriela Franco Domingos dos Santos [1]; Ana Rute Santos [2]; Peter Licence [2]; Luiz S. Longo Jr. [1]
[1] Universidade Federal de São Paulo/Departamento de Ciências Farmacêuticas; [2] The University Of Nottingham

The study of Sc(OTf)3 immobilized into polymer-supported ionic liquid phases (PSIL) as heterogeneous catalysts for the cyanosilylation of carbonyl compounds is described. The advantages of our method

Selênio e Pilar[n]arenos: da iniciação científica à formação de um grupo de pesquisa. Artigos, premiações e o dia a dia da ciência brasileira

https://proceedings.science/p/120654

Vanessa do Nascimento [1]

[1] Universidade Federal Fluminense - UFF

Esta apresentação traz um pouco da trajetória acadêmica da professora Vanessa Nascimento, desde sua iniciação científica até a formação do grupo de pesquisa SupraSelen. O intuito é mostrar a bagagem química que vem sendo desenvolvida por ela e por seus alunos atualmente. A história começa desde o período da sua iniciação científica na UFSM, passando pela pós graduação na UFSC e UNIPG (Itália) até os dias de hoje, como professora e pesquisadora na UFF. Tudo isso vem acompanhado de uma explicação dos principais artigos publicados pela mesma, bem como um pouco da narrativa de como as coisas aconteceram. O propósito é que o participante se inspire e melhor se direcione na construção de sua carreira acadêmica e na ciência.

Sequencial Mannich Synthesis of 1,4-Naphthoquinones and Evalution Against Oral Squamos Cells

https://proceedings.science/p/119418

Mariana S. S. M. Pereira [1]; Luana Forezi [1]; Michele Souza [1]; Ruan Carlos Ribeiro [1]; Bruno Kaufmann Robbs [1]; Vitor Ferreira [1]; Fernando de Carvalho [1]

[1] Universidade Federal Fluminense

Naphthoquinones obtained in sequential Mannich reaction. New synthetic methods that involve multicomponent reactions. Oral squamous cells carcinoma is in the sixth most incident cancer in the world.

SÍNTESE DE 3-(4-(FENILTIO)PIRIMIDIN-2-IL)IMIDAZO[1,2-a]PIRIDINA VIA REAÇÃO DE ATIVAÇÃO C-H EMPREGANDO UM CATALISADOR DE NÍQUEL

https://proceedings.science/p/120440

José Manuel da Cruz Tavares Junior [1]; Beatriz Amaral Lopes da Silva [1]; Beatriz Fuzinato dos Santos [1]; Estéfani Tayara Barce dos Santos [1]; João Paulo Bejamin dos Anjos [1]; Nelson Luis Campos Domingues [1]

[1] Universidade Federal da Grande Dourados

In this work, presents a methodological development of a C-H activation reaction for the synthesis of compound 3-(4-(phenylthio)pyrimidin-2-yl)imidazo[1,2-a]pyridine using Ni(mob) as a nickel catalyst

Síntese de glitazonas peptóides via reação de Ugi utilizando irradiação de microondas em um processo rápido, brando e escalável

https://proceedings.science/p/120584

Yuri Renan Braga Sousa [1]; Carlos Eduardo de Melo Salvador [1]; Carlos Kleber Z. Andrade [1]

[1] Universidade de Brasília

In only 4 linear steps, new peptoid glitazones with potential anticancer activity could be rapidly obtained, in good yields.

Síntese de novas N-alquil carboxamidas derivadas da 6-nitro-4-oxoquinolina para aplicação como intermediários sintéticos.

https://proceedings.science/p/120329

Mayra Silva Coutinho [1]; Kamili F. Ferreira [1]; Fernanda da Costa Santos Boechat [1]; Pedro Batalha [1]; Maria Cecília B. V. de Souza [1]

[1] Universidade Federal Fluminense

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Síntese de S-nitrosotióis terciários e ação anti-tumoral em linhagens humanas de câncer de mama

https://proceedings.science/p/120649

ADRIANA KARLA Cardoso Amorim Reis [1]
[1] Universidade Federal de São Paulo

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Síntese e avaliação anticorrosiva de iminas (2-N-amino-3-N-fenetilmetilenopiridina)

https://proceedings.science/p/120083

Ana Carolina Lima da Cruz [1]; Mariana Falcão Lopes Princisval Carlos [2]; Aurea Echevarria [1]; Cláudio Eduardo Rodrigues Santos [1]
[1] UFRRJ; [2] Universidade Federal Rural do Rio de Janeiro

As bases de Schiff estão presentes tanto nas atividades biológicas quanto na produção de novos materiais, e são conhecidas por apresentarem atividade anticorrosiva. A corrosão é um dos principais problemas encontrados no cotidiano, seja no meio industrial ou fora dele, e é caracterizada pela deterioração de diversos materiais, causando danos permanentes à sua superfície e, o prejuízo causado por corrosão é na ordem de bilhões[1]. Diante da importância de buscar novos inibidores anticorrosivos, este trabalho propõe uma síntese eficiente de bases de Schiff e relata sua atividade anticorrosiva utilizando a técnica de perda de massa. A síntese foi realizada a partir da condensação entre 2,3-diamino-5-bromo-piridina (1a) ou 2,3-diamino-piridina (1b) e salicilaldeído (2) utilizando água como solvente a uma temperatura 100 ◦C por 1 hora e 30 minutos (Figura 1), para a síntese do 3a e utilizando etanol como solvente por 3 horas para a síntese do 3b. Após este período a mistura foi filtrada, lavada com solvente, o produto sintetizado, recristalizado em etanol. Os rendimentos obtidos foram de 82 % e 62 % para os compostos 3a e 3b, respectivamente. Figura 1. Esquema de síntese das Bases de Schiff Os ensaios, para avaliação preliminar da atividade anticorrosiva dos compostos, foram realizados em placa de aço carbono AISI 1020, utilizando o ácido sulfúrico 1 mol L-1 como meio corrosivo nos períodos de 3 h e 6 h. Os compostos 3a e 3b foram testados na concentração de 10-2 mol L-1. Os resultados obtidos foram satisfatórios, tendo em vista que a síntese dos compostos foi realizada em água, um solvente verde, além disso, apresentou bons rendimentos. E, a inibição da atividade anticorrosiva do composto 3a foi de 93% nos tempos de 3 e 6 h e do composto 3b 87%, em ambos os tempos de imersão, a partir dos resultados pode-se observar que não houve diferença significativa nos tempos avaliados referentes a cada composto. Entretanto, o composto 3a, se mostrou mais eficiente que o 3b. Em termos estruturais, pode-se observar que, para esta classe de compostos, o bromo foi importante para a atividade anticorrosiva.

Síntese e avaliação das atividades citotóxica e leishmanicida de cinamatos derivados da vanilina

https://proceedings.science/p/120477

Bianca Ferreira da Silva [1]; Robson Ricardo Teixeira [2]; Raoni Pais Siqueira [2]; Gustavo Costa Bressan [3]; Wallace Pacienza Lima [4]
[1] Universidade Federal de Viçosa / Departamento de Química; [2] Universidade Federal de Viçosa; [3] Universidade Federal de Viçosa / Departamento de Bioquímica e Biologia Molecular; [4] Unigranrio.

The focus of this work was to synthesize of new molecular hybrids from vanillin and cinnamic acid derivatives and evaluate their cytotoxic and leishmanicide activities.

Síntese e caracterização de iminas contendo núcleo aminoquinolínico para posterior investigação da atividade biológica.

https://proceedings.science/p/119986

Talia Farias de Oliveira [1]; Edriane Teixeira da Silva [1]; Dimas J. da Paz Lima [1]; Mario Roberto Meneghetti [1]
[1] Universidade Federal de Alagoas

Na química medicinal e sintética os derivados quinolínicos representam um importante papel na síntese de novos fármacos contendo heterocíclicos de reconhecida aplicação biológica. Iminas são o produto da condensação de uma amina primária com um aldeído ou cetona, que também tem apresentando conter diversas e interessantes propriedades biológicas, como atividade antibacteriana, anti-inflamatória, antimicrobiana, leishimanicida, antimalárica e antitumoral1. Nesse contexto, o presente trabalho teve como propósito sintetizar uma série de compostos 4-aminoquinolinicos, contendo a função imina, e testá-los para possível atividade biológica, leishimanicida e antimalárica. Para a síntese desses derivados foi necessário preparar a N-(2-aminoetil) -7-cloroquinolin-4-amina (CEQ) a qual foi obtida, em 95% de rendimento, através da reação entre a 4,7-dicloroquinolina e etilenodiamina (Esquema 1). Posteriormente, a CEQ foi tratada com aldeídos aromáticos substituídos com grupos doadores e retiradores de elétrons na posição para fornecendo as iminas contendo o núcleo aminoquinolínico, em rendimentos que variaram entre 40 e 80%. Os compostos sintetizados foram caracterizados por IV, RMN de 1H e de 13C e serão encaminhadas para posterior investigação da citotoxidade e da atividade leishmanicida e antimalárica.

Síntese e caracterização de ligantes imidazolínicos

https://proceedings.science/p/120459

Elisângela Vinhato [1]; Ariadne de Jesus Vicente [1]; Alessandro Rodrigues [1]; Brenda Regina Bondezan Pereira [1]
[1] Universidade Federal de São Paulo

Synthesis of four N-Boc-imidazoline ligands derived from (1R, 2R)−1,2-diphenylethane-1,2-diamine. Ligands obtained with global yield from 52% up to 81%.

Síntese e caracterização de novos híbridos aciclonucleosídeos fosfonatos triazolil-4-quinolônicos.

https://proceedings.science/p/120325

Alan Gonçalves de Souza [1]; Claudio Santana Viana Junior [2]; Thaís Apolinário Tavares [2]; Letícia Villafranca Faro [2]; Marcos Costa de Souza [2]; Fernanda da Costa Santos Boechat [1]; Maria Cecília B. V. de Souza [2]
[1] Universidade Federal Fluminense; [2] Departamento de Química Orgânica / Instituto de Química / Universidade Federal Fluminense

ANPs such as HPMPC and PMEA have been identified as broad-spectrum antiviral agents but also offer great potential as antitumor agents. The search for new anticancer agents is a constant target.

Síntese, caracterização e análise de difração de monocristal das 2,3-Dipirazinilquinoxalinas e 2,3-Diimidazolquinoxalinas

https://proceedings.science/p/120628

Chárbel Carlos Ferreira Fontes [1]; Carolina Ligiéro [2]; Paulo Cesar Muniz de Lacerda Miranda [1]
[1] Universidade Estadual de Campinas; [2] Universidade Federal do Rio de Janeiro

Synthesis, characterization, and X-ray-crystallography analysis of new quinoxalines and their intermediates. Uncommon binding mode modes in solid state revealed by DRX.

Stereocontrolled Synthesis of Biogeosteranes: 3-(ω-(Methoxycarbonyl)alkyl) cholestanes - Molecular Fossils from the Cretaceous Period

https://proceedings.science/p/120547

Christian Rocque Maior [1]; Paulo Cesar Muniz de Lacerda Miranda [1]
[1] Universidade Estadual de Campinas

Synthesis of 3-(ω-(methoxycarbonyl)alkyl)cholestanes from olefin metathesis and kinetic or thermodynamic controlled hydrogenations furnished three homologs for each 3,5 possible configurations.

Studies aiming the obtaining of Camphor O-benzyl-oxime derivatives with potential biological activity

https://proceedings.science/p/119740

Gabriel Andrade [1]; Emerson da Silva [2]; Marcus Souza [2]
[1] Faculdade de Farmácia - UFRJ / Instituto de Tecnologia em Fármacos - Fundação Oswaldo Cruz; [2] Fundação Oswaldo Cruz

Camphor oxime derivatives were synthesized in a mixture of an aqueous solution of NaOH and ethanol.

The reactions were conducted under ultrasound irradiation and fast reaction time.

Studies for the stereoselective synthesis of (-)-cleistenolide by controlling stereocenter from D-mannitol

https://proceedings.science/p/120110

Suélen Karine Sartori [1]; Marisa Alves Nogueira Diaz [2]; Gaspar Diaz-Muñoz [1]
[1] Universidade Federal de Minas Gerais/Departamento de Química; [2] Universidade Federal de Viçosa (UFV - Campus Viçosa)

(-)-Cleistenolide is a remarkable natural product in the 5,6-dihydropyran-2-one class, of great pharmacological interest due to its antibacterial activity against Staphylococcus aureus and antifungal against Candida albicans.1,2 It was isolated in 2007 from Cleistochlamys kirkii, a plant originally from Tanzania and Mozambique.3 Due to its pharmacological potential3,4, this study aims to develop a new concise synthetic route for obtaining this natural d-lactone from D-mannitol. This approach tries to take advantage of the correct stereogenic centers already established in sugar in order to transfer them to the target molecule. The synthesis of (-)-cleistenolide begins with the preparation of triacetonide 1 from D-mannitol by treating it with acetone under acid catalysis, followed by a regioselective deacetylation step to provide acetonide-diol 2 (Scheme 1). Oxidative cleavage of the diol, followed by modified Horner-Wadsworth-Emmons olefin reaction5 of the resulting aldehyde with phosphonate 4 (prepared in our laboratory) provided olefin 5 with dr: (Z:E) 94:6, stereochemistry required to promote lactonization. Regioselective deacetalization from 5, followed by mono-protection of the primary hydroxyl with TBDPS led to the formation of the alcohol ester 7, a key intermediate with all controlled stereocenters for the total synthesis of the molecule. This was converted into its respective carboxylic acid by the use of LiOH, which was subjected to the cyclization step using FeCl3.6H2O6,7 to form the respective g-lactone 9 with 78% yield (Scheme 1). Subsequently, the hydroxyls' protection step as silyl ethers, followed by a trans-silylation protocol, should promote the conversion of the g-lactonic ring into d-lactonic ring. Deprotection and monoprotection steps with a benzoyl group, followed by acetyl will make it possible to obtain (-)-cleistenolide. The proposed synthetic route made it possible to obtain dihydroxy g-lactone 9, an advanced intermediate to produce (-)-cleistenolide. The latter and the previous intermediates were properly characterized by 1H and 13C NMR.

SUSTAINABLE SYNTHESIS OF ISATIN DERIVATIVES AND EVALUATION IN ACIDIC MEDIUM AS CORROSION INHIBITORS

https://proceedings.science/p/120615

CAROLAINE SILVA [1]; Cláudia Moreira de Mesquita [1]; Anna Cláudia Cunha [1]; Eduardo Ariel Ponzio [1]; Vinicius Campos [1]
[1] Universidade Federal Fluminense

This work describes the sustainable synthesis of three isatin derivatives with semicarbazonic, tiossemicarbazonic and aminoguanidine moiety. The corrosion inhibition was evaluated by weigt loss method

Synthesis and antioxidant activity of polyfunctionalized organoselenides employing a seleno-containing cyanohydrin as building block

https://proceedings.science/p/120486

Juliana Thomas [1]; Leandro Piovan [1]
[1] Universidade Federal do Paraná

A simple route to synthesize polyfunctionalized organoselenides from Se-cyanohydrin was developed. Some of them presented promising in vitro antioxidant activity.

Synthesis and antitumor evaluation of trifluoromethyl aryl diamides

https://proceedings.science/p/119588

Michelle Rodrigues Peixoto [1]; Robson Ricardo Teixeira [1]; Raoni Pais Siqueira [1]; Gustavo Costa Bressan [1]; Giovanni Amarante [2]
[1] Universidade Federal de Viçosa; [2] Universidade Federal de Juiz de Fora
It is herein described the preparation of a series of trifluoromethyl aryl diamides and the evaluation of their activity against HeLa, HepG2 (tumor cells) and HEK 293 (non-tumor cells).

Synthesis and application of new organotellurium-pillar[5]arene as catalysts for halogenation reaction

https://proceedings.science/p/119523

Beatrice Faria de Almeida Barboza Brasil [1]; Ingrid Cavalcanti Chipoline [2]; Vanessa do Nascimento [2]
[1] Universidade Federal Fluminense -UFF; [2] Universidade Federal Fluminense - UFF
Pilar[5]arenes and organotellurium compounds are described as effective catalysts in many organic reactions. This study presents the synthesis and application of a new organotellurium-pillar[5]arene.

Synthesis and application of pillar[5]arenes as corrosion inhibitors

https://proceedings.science/p/119954

Amanda Rebelo de Azevedo [1]; Pâmella da Silva Cordeiro; Vanessa do Nascimento [2]; MATHEUS PRADO [3]; Caio M. Fernandes [1]; Eduardo A. Ponzio [1]
[1] UFF - UNIVERSIDADE FEDERAL FLUMINENSE; [2] Universidade Federal Fluminense - UFF; [3] Universidade Federal Fluminense
Design and synthesis of pillararenes functionalized with nitrogen compounds with high potential for anti-corrosion activity.

Synthesis and Biological Prospection of Naphthoquinone Hybrids Containing 1,2,3-Triazolic Linked as Potential Anticancer Drugs

https://proceedings.science/p/120073

Acácio Silva de Souza [1]; Ruan Carlos Ribeiro [2]; Matheus Gonzaga de Moraes [3]; Maria Eduarda Globa Masset [4]; Fernando de Carvalho [2]; Vitor Ferreira [4]
[1] Universidade Federal Fluminense, Departamento de Tecnologia Farmacêutica; [2] Universidade Federal Fluminense; [3] Universidade Federal Fluminense / Departamento de Química Orgânica, Instituto de Química; [4] Universidade Federal Fluminense / Departamento de Tecnologia Farmacêutica, Faculdade de Farmácia

It is a search for new hybrids with a good relationship between structure and activity. Thus, it is intended to investigate how the junction of such systems may influence the anticancer activity.

Synthesis and characterization of N-acetylacetamido-1H-1,2,3-triazole derivatives

https://proceedings.science/p/120045

Thais de Brito da Silva [1]; Kathya Ng Ka Ji [1]; Luana Forezi [1]; Vinicius Campos [1]; Fernando de Carvalho da Silva [1]; Vitor Ferreira [1]

[1] Universidade Federal Fluminense

This work describes the synthesis of diacetyl-triazoles, which were obtained via the diacetylation of amino-triazole derivatives in the presence of acetic acid, pyridine and DMAP as a catalyst. Diacetyl compounds have recently attracted significant interest due to their broad spectrum of biological activities such as anticancer, herbicide, antifungal, anti-ulcer and anti-secretory. The methods for the preparation of diacetylamines, in specific, involve the reaction of amines with acetylating agents such as acetyl chloride, acetic anhydride, and ketene and enol esters in the presence of catalysts such as pyridine, sulphuric acid, and sodium acetate.In this work, ethyl 5-amino-1H-triazole-4-carboxylate derivatives were obtained from the reaction between phenylazides and ethyl cyanoacetate in the presence of sodium ethoxide at room temperature for 3 hours. Then, the ethyl 5-amino-1H-triazole-4-carboxylate derivatives were reacted with acetic anhydride, pyridine and DMAP as the catalyst at room temperature for 24 hours to form nine new N-diacetyl derivatives. All synthesized compounds were characterized using H1- and C13-NMR, as well as high resolution mass spectrometry.

Synthesis and characterization of novel pyrrolobenzodiazepines-1H-1,2,3-triazoles derivatives as potent anticancer agents

https://proceedings.science/p/120002

Sabrina Baptista Ferreira [1]; Floriano Silva-Jr [2]; Dinesh Addla [3]; Tereza Cristina Santos Evangelista [4]; Carlos R. Kaiser [3]; Rafael Dantas Ribeiro [2]

[1] Universidade Federal do Rio de Janeiro - UFRJ; [2] Fiocruz; [3] UFRJ; [4] IQ-UFRJ

Pyrrolo[2,1-c][1,4]benzodiazepines (PBD) are a class of naturally occurring tricyclic molecules that exhibit a broad spectrum of biological activities, featuring its antitumor properties. Currently, some efforts have been made on the synthesis of new PBD derivatives linked with different units, including heterocycles and aliphatic chains.1 In this manner, the present work proposed the synthesis of new PBD-triazole derivatives as new antitumor agents. The 1,2,3-triazole synthesis will be carried out by the copper-catalyzed 1,3-dipolar cycloaddition (CuAAC) reaction, between different commercial aliphatic and aromatic alkynes and the azido-PBD key derivative. The PBD-triazoles were synthesized according to the Scheme 1, starting with a condensation reaction between isatoic anhydride (1) and trans-hydroxy-L-proline (2) affording the PBD-alcohol (3), followed by the conversion of the hydroxyl group into a better leaving group (4). After that, a SN2 reaction with NaN3 in DMF affords the azido-PBD derivative (5). To afford the PBD-triazoles, the CuAAC reaction was tested under different reaction conditions, including the use of an ultrasonic bath and reflux. However, the most promising results were obtained when the reaction was carried out in a microwave, at 115 C, for 15 min. The reactions proved to be efficient and the products were easily isolated, being purified by column chromatography affording the new PBD-triazoles (6a-p). Structural elucidation of the compounds was performed by IR, 1H, 13C NMR and HRMS. Currently, the novel compounds are under biological evaluation as anticancer agents against different panels of cancer cells.

Synthesis and characterization of novel sulfonamide-sydnone hybrids as potential cytotoxic agents

https://proceedings.science/p/119875

Igor Resendes Barbosa [1]; William Queiroz Felippe [1]; Ana Paula Pereira da Silva [1]; Aurea Echevarria [1]

[1] Universidade Federal Rural do Rio de Janeiro

New sulfonamide-sydnone hybrids were successfully synthesized by a five-step route, characterized by spectroscopic methods (IR, 1H and 13C NMR) and evaluated against a liver cancer cell line (HepG2).

Synthesis and evaluation of antiproliferative activity of quinazoline-chalcone hybrids

https://proceedings.science/p/120605

Gilmar Vieira Duarte [1]; Eduardo Bustos Mass [2]; Erick Urban Bueno Alvares [1]; Carolina Lima [3]; Giovanna Barbarini Longato [3]; Dennis Russowsky [1]; Carolina Afonso de Lima [4]

[1] Universidade Federal do Rio Grande do Sul; [2] Universidade Federal do Rio Grande do Sul/ IQ (Instituto de Química); [3] Universidade São Francisco; [4] Universidade São Franscisco

The new hybrid molecules were obtained fast and easily in reasonable yields; Hybrid 5a,b were more potent than Doxorubicin

Synthesis and evaluation of new pyridine-marinoquinolines as antimalarials

https://proceedings.science/p/119858

Rebeca Monique Capitão [1]; Rafael Dias do Espírito Santo [1]; Guilherme Eduardo de Souza [2]; Rafael Victorio Carvalho Guido [2]; Carlos Roque Duarte Correia [1]

[1] Universidade Estadual de Campinas; [2] Universidade de São Paulo

3H-pyrrolo[2,3-c]quinoline is a tricyclic system rare between natural products. The first example reported was Marinoquinoline A, isolated from the gliding bacterium Ohtaekwangia kribbensis together with the novel marinoquinolines B-F. These compounds have demonstrated activity as acetylcholinesterase inhibitor, antibiotic activity, antitumoral and antiprotozoatic. In view of the pharmacological potential of marinoquinolines, the present work describes the moldular synthesis of novel marinoquinolines. Pyrroloanilines intermediates were synthesized by Suzuki-Miyaura cross-couplings followed by Pictet-Spengler cyclizations to obtain the desired pyridine-marinoquinoline in good overall yields.

Synthesis and evaluation of the antibacterial activity of 1,4-naphthoquinone linked to sulfonamides

https://proceedings.science/p/120086

Marcela Cristina Pereira de Barros [1]; Daniel Tadeu Gomes Gonzaga [2]; Vitor Ferreira [1]; Fernando de Carvalho da Silva [1]; Paulo A. F. Pacheco [1]

[1] Universidade Federal Fluminense; [2] UEZO

Naphthoquinones are natural and synthetic products that have the ability to generate reactive oxygen species (ROS) through a redox mechanism. This process involves the presence of anions, dianions, superoxide anions and semiquinone radicals that can cause intracellular hypoxia leading to oxidative stress and, consequently, cell death. As a consequence, synthetic and natural naphthoquinones exhibit a sum of biological activities, including antibacterial activity. Sulfonamides are structural analogues of p-aminobenzoic acid (PABA), which inhibits folic acid metabolism, an essential factor for bacterial growth. In addition, structural insertions in the sulfonamide structure allowed an extension of its pharmacological applications. Considering these factors, in this work, we synthesized 1,4-naphthoquinones linked to sulfonamides containing a 1,3-phenylene diamamine linker in order to obtain new new compounds with potential antibacterial activity. To obtain the planned antibacterial compounds, aminonaphtoquinone 1 was reacted with different sulfonyl chlorides 2a-e, thus leading to compounds 3a-e. All compounds had their chemical structures confirmed by hydrogen nuclear magnetic resonance (1H and 13C-NMR), infrared and high resolution mass spectroscopy (HSMRS).

Synthesis and photophysical characterization of flavylium and pyranoflavylium salts

https://proceedings.science/p/120314

Fabiana Cristina Lopes [1]; Vinícius Viana Marto [1]; Cássio Pacheco Silva [2]; Frank Herbert Quina [2]; Vânia Maria Teixeira Carneiro [1]

[1] Universidade Federal de Viçosa - Campus Viçosa; [2] Universidade de São Paulo

Novel flavylium and pyranoflavylium salts were synthesized.
Photophysical characterizations were conducted in three different solvents.

Synthesis and photophysical properties of new 6-amino-2-alkyl(aryl/heteroaryl)-4-(trifluoromethyl)quinolines

https://proceedings.science/p/119511

Yuri Giovane Kappenberg [1]; Helio Bonacorso [1]; Bernardo Almeida Iglesias [1]; Thiago V. Acunha [1]
[1] Universidade Federal de Santa Maria

A new series of 6-amino-4-(trifluoromethyl)quinoline scaffolds was easy synthesized and the promising photophysical properties in solution has been demonstrated.

Synthesis and structure determination of 2-amino-naphthoxazoles prepared from β-lapachone: comparison of theoretical and experimental spectral data.

https://proceedings.science/p/120222

Luan Matheus da Silva Freire [1]; Aurélio Baird Buarque Ferreira [1]; Leonardo Araujo Silva [1]; Emanoel Hottes [1]; Ari Miranda da Silva [2]; Guilherme Pereira Guedes [3]; Marcelo Herbst [1]; Jefferson Yoshinaga [1]
[1] Universidade Federal Rural do Rio de Janeiro; [2] Universidade Federal do Rio de Janeiro; [3] Universidade Federal Fluminense

The present work reports the synthesis of two 2-amino-naphthoxazoles and the experimental and thoretical studies aiming their characterization, including, in one case, X-ray diffraction.

Synthesis of 1,4-naphthoquinone/thiophene scaffolds aiming the search for new anticancer agents

https://proceedings.science/p/120024

Mariana de Castro Gonçalves [1]; Daniel Tadeu Gomes Gonzaga [2]; Fernando de Carvalho da Silva [3]; Vitor Ferreira [3]; Gabriel Oliveira de Resende [4]
[1] UFF; [2] UFAR / CCBS / UEZO; [3] Universidade Federal Fluminense; [4] Núcleo de Ciências Químicas / Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro

The synthesis of 1,4-naphthoquinones conjugated to the thiophene nucleus was achieved using different 1,4-naphthoquinones and acyl chlorides containing the thiophene nucleus in their structure. Considering the pronounced activity of the isolated scaffolds, it is possible that a synergistic anti-cancer action takes place.

Synthesis of 1H-1,2,3-triazoles conjugated to the thiophene nucleus with potential anti-inflammatory activity

https://proceedings.science/p/119997

Danielle Pagliaminuto Portella [1]; Daniel Tadeu Gomes Gonzaga [2]; Dora Costa [3]; Fernando de Carvalho [4]; Danielle Montenegro da surreição [2]; Vitor Ferreira [1]; Maria Eduarda L. de Lima [2]
[1] UFF; [2] UEZO; [3] Universidade de Aveiro (Portugal); [4] Universidade Federal Fluminense

Resumo/Abstract The 1H-1,2,3-triazole consists of a five-membered heterocyclic ring containing three adjacent nitrogens atoms. The triazole are an important pharmacophoric group found in important drugs such as the beta-lactam antibiotics tazobactam and cephalosporin cefatrizine.1 Additionally, there are reports of numerous biological activities such as antiviral, antichagasic and, anti-inflammatory, among others.2 On the other hand, the thiophene nucleus consists of a five-membered aromatic ring which, contains sulfur as a heteroatom. This moiety is also well-consolidated in medicinal chemistry, with several drugs presenting the thiophene ring in their chemical skeleton, e.g. of clopidogrel, an antiplatelet agent.3 In addition to drugs, there are several reports of such compounds as displaying varied biological properties that include antimicrobial and anti-inflammatory activity, among others.4 In this sense, in this work we envisioned the combination of these two nuclei in order to study the occurrence of at a possible synergistic anti-inflammatory action. The methodology used for the synthesis of such compounds consists in the acylation of the triazole alcohol (R=H, R=4Cl, R= 2,5diCl, R=3,4diCl, R=4-NO2, R=4-OCH3, R=4-F, R=4-CH3) with the 2-thiophene acyl chloride (2a-b) catalyzed by DMAP, in the presence of pyridine as a base. All compounds were obtained with yields ranging from moderate to quantitative. The chemical structures were elucidated using nuclear Magnetic resonance (1H and 13C NMR), Fourier-transform infrared (IR) and high-resolution mass spectrometry (HRMS). 1-Melo; J. O. F., Donnici, C. L., Augusti, R., Ferreira, V. F., Souza, M. C. B. V., Ferreira, M. L. G. and Cunha, A. C. (2006), Química Nova, 29 (3), 569-579. / 2-Agalave, S. A., Maujan, S. R. and Pore, V. S. (2011), Chemistry Asian Journal 6, 2696 – 2718./ 3- Lahsasni, S, Al-Hemyari, D. A. M., Ghabbour, H. A., Mabkhoot, Y. N., Aleanizy, F. S., Alothman, A. A.

and Almarhoon1, Z. M. (2018), Journal of Chemistry, Volume 2018, Article ID 8536063, 11 pages. / 4- Chaudhari, P. S.,Chitlange, S. S. and Nanda, R. K. (2018), Anti- Inflammatory & Anti-Allergy Agents in Medicinal Chemistry, 17, 102-114.

SYNTHESIS OF 2-FENIL-3-(FENILSELANIL)BENZOFURANO IN ENVIRONMENTALLY SUITABLE CONDITIONS

https://proceedings.science/p/119642

Matheus Prado [1]; Pâmella da Silva Cordeiro; José S. S. Neto [2]; Vanessa do Nascimento [3]; Antônio L. Braga [2]
[1] Universidade Federal Fluminense ; [2] Universidade Federal de Santa Catarina; [3] Universidade Federal Fluminense - UFF

This project deals the design and synthesis of selenobenzofurans carried out through green chemistry protocols, which main to reduce or eliminate the use and generation of dangerous substances.

Synthesis of a Novel Chiral Catalyst Based on Thioproline and Thiourea to be applied in Asymmetric Michael Reaction

https://proceedings.science/p/119917

Flavia Rodrigues Alvares [1]; Frederico Ricardo Castro Noronha-Jr [1]; Tiago Lima da Silva [1]; Sabrina Baptista Ferreira [1]
[1] Universidade Federal do Rio de Janeiro - UFRJ

Bifunctional catalysts based on thiourea have shown to be efficient in promoting asymmetric reactions. In this work we propose the development of an asymmetric methodology to afford a library of Michael adducts.

Synthesis of acrylics acid derivatives: a simple, multigram scale, sonochemical synthesis.

https://proceedings.science/p/120301

Letícia Bárbara Silva da Penha [1]; Marcus Souza [2]; Victor Facchinetti Luz [3]
[1] Universidade Federal Fluminense ; [2] Fundação Oswaldo Cruz; [3] Fiocruz

Four Acrylic acid derivatives with high added-value were synthesized in 35-90% yields by a simple and efficient multigram scale methodology via sonochemistry, in 1h, after easy work-up.

Synthesis of amides containing benzylpiperazine: potential agents against tuberculosis.

https://proceedings.science/p/119645

Claudia Regina Brandão Gomes [1]; Rafael Dantas Ribeiro [2]; Cristiane França da Costa [3]; Marcus Vinicius Nora de Souza [1]
[1] Fundação Oswaldo Cruz; [2] IFRJ, Departamento de Síntese de Fármacos / Farmanguinhos / Fiocruz; [3] Fiocruz

Tuberculosis (TB) is a global emergency, launching a joint effort to mobilize resources to fight the epidemic. However, new substances have been promising in view of this situation.

Synthesis of benzofurans by one-pot Wittig-Friedel-Crafts reactions

https://proceedings.science/p/119697

Fernando Alves Barretto [1]; SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

Benzofurans were obtained by short synthesis of phosphorus ylide and furfuraldehyde via Wittig and Friedel-Crafts reaction.

Synthesis of bis-aldiminas as potentials soil urease inhibitors

https://proceedings.science/p/119428

Anna Luísa Lacerda de Almeida Sousa [1]; Luzia Valentina Modolo [2]; Sergio Antonio Fernandes [1]
[1] Universidade Federal de Viçosa; [2] Universidade Federal de Minas Gerais

In the present work, the synthesis of bis-aldimines as potential soil urease inhibitors has been developed. Ureases are part of a class of enzymes that catalyze the hydrolysis of urea to the formation of ammonia, water and carbon dioxide. Despite the low cost, urea when applied to the soil, suffers loss of nitrogen by volatilization when hydrolyzed. With this limitation, the development of potentials urease inhibitors is fundamental, since the national market does not have this technology. Aldimines, inspired by the reaction between tiocarbohydrazone and aldehydes, may be an alternative as urease inhibitors due to structural similarity with thiourea to bypass large nitrogen losses through the hydrolysis of urea. Were synthesized eight bis-aldimines, which were purified by recrystallization and the yields ranging from 46 to 89%.

Synthesis of bis-imines thiazoles using multicomponent reactions

https://proceedings.science/p/119479

Amanda Oliveira Barros [1]; Sergio Antonio Fernandes [1]
[1] Universidade Federal de Viçosa

Thiazoles are heterocycles compounds with five membered ring that contain three carbon atoms, one sulphure atom and one nitrogen atom. Recently, the synthesis of bis-imines by multicomponent reaction was reported using thiocarbohydrazide, a ketone and an aromatic aldehyde. Multicomponent reactions combine elements of an ideal synthesis such as operational simplicity and atom economy, in addition to that there is also the reduced number of steps. This molecules were synthesized from thiocarbohydrazide (0.5 mmol), an aromatic aldehyde (2 mmol) and 2-bromoacetophenone (0.5 mmol), using p-sulphonic acid calix[4]arene as the catalyst. The interest in bis-imines thiazoles is due to some biological activities already reported in the literature such as antituberculosis, antibacterial, antimalarial, antifungal, inhibitors of human monoamine oxidase A and B enzymes and antitumor. Six bis-imines thiazoles have been synthesized in yields ranging from 12% to 70%.

Synthesis of different molecules from furfural using niobium compounds as catalysts of reactions

https://proceedings.science/p/119698

Aline Nakagawa do Nascimento [1]; Camila Oliveira [1]; Messias Cardoso Loiola [1]; Victor dos Santos Pinheiro [1]; Mauro Coelho dos Santos [1]; Bruno Lemos [1]; Mirela Sairre [1]
[1] Universidade Federal do ABC

Furfural can be obtained from hydrolysis of biomass. It was used in reactions for the synthesis of furanochalcones, dihydropyridines and dihydropyrimidinones.

Synthesis of Dihydropyridine-Dihydropyrimidinone hybrids via copper-catalyzed azide-alkyne cycloaddition reaction

https://proceedings.science/p/120571

Vanessa P. de Souza [1]; Camila D. Cesar [1]; Eduardo Bustos Mass [1]; Dennis Russowsky [2]
[1] Universidade Federal do Rio Grande do Sul/ IQ (Instituto de Química); [2] Universidade Federal do Rio Grande do Sul

• Fast and easy synthesis based on combined Multicomponent Reactions/Huisgen CuAAC
• New complex molecular architecture for biological multifunctional activity investigations

Synthesis of eugenol Schiff bases derivatives

https://proceedings.science/p/119578

Rosiene Mattos [1]; Silvio Cunha [1]
[1] Universidade Federal da Bahia

Schiff bases or imines and derivated were synthesized by formylation Duff with eugenol (1) then condensation reaction employing amines, hydrazines and hydrazones.

Synthesis of Fluorescent Benzothiadiazoles and Derived Hybrid Materials

https://proceedings.science/p/119922

Victória Goulart Isoppo; Marieli Rodrigues [1]; Lucas Zielinski do Canto [1]; Angélica Venturini Moro [1]; Fabiano Severo Rodembusch [1]
[1] Universidade Federal do Rio Grande do Sul

Photoluminescent silylated organic compounds have a wide range of applications, due to their potential in the development of new hybrid materials. The insertion of silicon opens the possibility of synthesis of organic-inorganic hybrid materials, which have different characteristics that can be superior to pure matrices. Due to its fluorescent characteristics, the benzothiadiazole nucleus can be used in the synthesis of organic-inorganic hybrid materials, since fluorophores can be incorporated in several inorganic matrices. Through the sol-gel methodology, organofunctionalized materials are synthesized, where the properties of the organic compound are combined with the thermal and mechanical stability of the inorganic compounds.

Synthesis of Lawsone from 2-amino-1,4-naphthoquinones

https://proceedings.science/p/119609

Igor Sande de Santana [1]; SILVIO CUNHA [1]
[1] Universidade Federal da Bahia

Lawsone was synthesized from hydrolysis of 2-phenylamino- and 2-amino-1,4-naphthoquinones. This synthesis was tested in one-pot reaction and in gram scale.

Synthesis of Molecular Hybrids with Potential Antitumoral Activity

https://proceedings.science/p/119505

Cláudia Laís Araújo Almeida Santos [1]; Jonh Anderson Macêdo Santos [2]; Paulo Henrique Menezes [1]
[1] Universidade Federal de Pernambuco; [2] Universidade Federal Rural de Pernambuco

An efficient approach for the synthesis of molecular hybrids containing Z-enynes and carbohydrate derivatives is described. The products were obtained in good to moderate yields in a stereoselective way.

Synthesis of naphthoquinoidal compounds with trypanocidal and antitumor activities

https://proceedings.science/p/120315

Renata de Almeida [1]; Renato Lúcio de Carvalho [1]; Gleiston Gonçalves Dias [1]; Eufrânio N. da Silva Júnior [1]
[1] UFMG

A variety of quinone-based 1,2,3-triazoles were synthesized by using click chemistry reactions, copper catalyzed azidealkyne 1,3-dipolar cycloaddition, and evaluated against six types of cancer cell lines: HCT-116 (human colon carcinoma cells), PC3 (human prostate cells), HL-60 (human promyelocytic leukemia cells), SF295 (human glioblastoma cells) and NCI-H460 (human lung cancer cells). Murine fibroblast immortalized cell lines (L929) were used to evaluate the selectivity of the compounds. These new methods provide efficient and practical strategies for the preparation of quinones. In addition, we have discovered compounds with potent trypanocidal activity.

Synthesis of Naphthoquinone-Triazole-Coumarin Hybrids and Evaluation Against Oral Squamous Cell Carcinoma

https://proceedings.science/p/120231

Amanda de Andrade Borges [1]; Luana Forezi [1]; Amanda Vieira Ribeiro [1]; Anna Fonseca [1]; Ruan Carlos Ribeiro [1]; Bruno Kaufmann Robbs [1]; Vitor Ferreira [1]; Fernando de Carvalho [1]

[1] Universidade Federal Fluminense

The search for new bioactive molecules begins with its relevance in the literature, as is the case of naphthoquinone, coumarin and 1,2,3-triazole systems, which have several individual biological properties. Thus, the objective of this work is to obtain new naphthoquinone-triazole-coumarin hybrids, and to evaluate how the combination of such systems can influence biological activity of these new molecules, more specifically in face of squamous cells of oral carcinoma (OSCC).

Synthesis of new 1,2,3-triazoles as new molecular Nutlin analogues

https://proceedings.science/p/120080

Fernanda Petzold Pauli [1]; Wislayanne Rodrigues Santos [1]; Vitor Ferreira [1]; Fernando de Carvalho [1]

[1] Universidade Federal Fluminense

The p53 protein plays a critical role in the regulation of the cell cycle and apoptosis. This protein is often inactivated in various types of human cancer by abnormally high levels of its negative regulator, the Minute Double Mourine 2 (MDM2). As a result, the reactivation of p53 function by inhibiting the protein-protein p53-MDM2 interaction has been pointed as a promising strategy for cancer therapy. In 2004, 1,2,4,5-tetrasubstituted-4,5-cis-imidazolines, also known as Nutlins, were discovered through high throughput screening at Hoffman-La Roche as potent MDM2 inhibitors. However, the stereogenic centers present in the structure of the Nutlins prevents the use of simple synthetic routes towards them, which promotes the search for new small molecule inhibitors of MDM2. In this context, the 1,2,3-triazole system has been extensively studied and used in medicinal chemistry. Considering the vast experience of our group in this field, the objective of this work was to synthesize 1,2,3-triazole compounds as new molecular analogues to the Nutlins family.

Synthesis of new 2-arylquinazoline-chalcone hybrids

https://proceedings.science/p/120580

Erick Urban Bueno Alvares [1]; Gilmar Vieira Duarte [1]; Eduardo Bustos Mass [2]; Dennis Russowsky [1]

[1] Universidade Federal do Rio Grande do Sul; [2] Universidade Federal do Rio Grande do Sul/ IQ (Instituto de Química)

New one-pot method to synthesize 4-aminoquinazolines from quinazolinones;
New set of hybrid compounds 2-arylquinazoline-chalcone in good yields;
Pure compounds(^{1}H NMR) easily obtained by decantantion.

Synthesis of new azido-glycero-pyrimidine derivatives

https://proceedings.science/p/119471

Carla Jasmine Oliveira e Silva [1]; Jóse Geovane Jorge de Matos [2]; Bruna Martins Guimarães [1]; Ronaldo Nascimento de Oliveira [1]

[1] Universidade Federal Rural de Pernambuco - UFRPE; [2] Universidade Federal de Pernambuco - UFPE

This work describes the synthesis of different glycero-pyrimidine derivatives linked to azide and triazole.

Synthesis of new cyclopentene-fused dihydropyridones through reaction of cyclic enaminone with coumarin-3-carboxylic acids

https://proceedings.science/p/120129

Iva Souza de Jesus [1]; Silvio do Desterro Cunha [2]
[1] Universidade Federal da Bahia; [2] Universidade Federal da Bahia

Herein, we describe the formal aza-[3+3] cycloaddition of cyclic enaminone 2 with coumarin-3-carboxylic acid derivatives 1a-i afforded cyclopentene-fused dihydropyridones 3a-i in good yields.

Synthesis of pillar[5]arenes derived from amino acids with potential application in asymmetric catalysis

https://proceedings.science/p/119603

Pâmella da Silva Cordeiro

Synthesis of prototypes with potential activity against Plasmodium falciparum: triazolopyrimidine derivatives

https://proceedings.science/p/120320

Endrew Moraes Amaral [1]; Cristiane França da Costa [2]; Luiz Carlos da Silva Pinheiro [2]; Núbia Boechat Andrade [3]
[1] Síntese de Fármacos / Farmanguinhos / Fundação Oswaldo Cruz; Instituto de Química / Universidade Federal do Rio de Janeiro; [2] Síntese de Fármacos / Farmanguinhos / Fundação Oswaldo Cruz; [3] Fundação Oswaldo Cruz

In this work 3 final products were synthesized with 55–77% yields and will be sent for testing against P. falciparum. These
compounds are promising for further studies as antimalarials.

Synthesis of γ-azido-α-diazo-β-hydroxy ester en route to O-acylated products through the Steglich esterification

https://proceedings.science/p/120152

Gabriela Maciel Diogo [1]; Marcus Sá [1]
[1] Universidade Federal de Santa Catarina

Synthesis of γ-azido-α-diazo-β-hydrox ester was achieved through the chemoselective reduction of the corresponding α-diazo-β-keto ester. Steglich esterification with carbodiimides a gave O-acylated analogues.

Synthesis, characterization and electrochemical polymerization of pyrrole derivatives for application in forensic chemistry.

https://proceedings.science/p/119458

Ana Carolina Fradique de Lyra [1]; Jorge de Lima Neto [1]; Luis Paulo Alves da Silva [1]; Adriana Santos Ribeiro [1]; Dimas José da Paz Lima [1]
[1] UFAL

- The synthesis, characterization and electrochemical polymerization of 4-(Pirrol-1-yl)-Butanoic Acid and Ethyl 4-(Pirrol-1-yl)-Butanoate Ester were achieved. - Development of fingerprints in metal.

The First Total Synthesis of Bhutkesoside A: Polyacetylenic Glycoside With Potential Anticancer Activity

https://proceedings.science/p/119484

Jonh Anderson Macêdo Santos [1]; Cláudia Laís Araújo Almeida Santos [2]; Paulo Henrique Menezes [2]; Juliano Carlo Rufino de Freitas [3]

[1] Universidade Federal Rural de Pernambuco; [2] Universidade Federal de Pernambuco; [3] Universidade Federal de Campina Grande

Polyacetylenic glycosides are derived from polyynes compounds, a class of natural products characterized by the presence of two or more conjugated triple bonds in their structure. These molecules are widely distributed in various medicinal plants. In 2015, Adhikari and coworkers reported the isolation of Bhutkesodide A from the roots of the Ligusticopsis wallichiana plant. Bhutkesodide A has shown promising antineoplasic activity. In addition, it is a potential inhibitor of uridine cytidine kinase 2 (UCK2), which is expressed in cancer cells, so this enzyme is an important biological target in cancer treatment. Thus, in this work we report the first total synthesis of Bhutkesodide A. A convergent synthesis of Bhutkesoside A was achieved after five reaction steps in 25% overall yield. The synthesized compounds were characterized by the usual spectroscopic techniques and the data corroborate the structures.

The one-pot Biginelli reaction/nitroaromatic reduction applied to the synthesis of quinazoline-dihydropyrimidinone hybrid

https://proceedings.science/p/120594

Eduardo Bustos Mass [1]; Erick Urban Bueno Alvares [2]; Dennis Russowsky [2]

[1] Universidade Federal do Rio Grande do Sul/ IQ (Instituto de Química); [2] Universidade Federal do Rio Grande do Sul

-Novel one-pot Biginelli reaction/nitroaromatic reduction in higher yields than conventional two steps reaction;
-H NMR-pure compounds easily crystallized from ethanol;
-New quinazoline-DHPM hybrid.

The search for organosulfurated sustainably-obtained bioactive compounds

https://proceedings.science/p/119807

Rafaella Garcia Angelino [1]; Vanessa do Nascimento [2]; Luana da Silva Gomes [1]

[1] Universidade Federal Fluminense; [2] Universidade Federal Fluminense - UFF

This work presents a range of sulfur-functionalized alkenes obtained through a simple and eco-friendly methodology.

The second-generation synthesis of the URAT1 inhibitor Lesinurad

https://proceedings.science/p/119796

Julio Pastre [1]; Mariana Damião [2]; Henrique Marçon [2]

[1] UNICAMP; [2] Unicamp

Lesinurad, a URAT1 inhibitor, is used for treating high blood uric acid levels associated with gout. In the present work, we developed a more cost- and time-effective synthesis of lesinurad using a continuous flow platform.

The Steglich Rearrangement of Azlactones and Isoxazolones: a Theoretically-Driven Experimental Investigation

https://proceedings.science/p/120316

Pedro Pôssa de Castro [1]; Juliana Alves dos Santos [1]; Marcelo Magno de Siqueira [1]; Gabriel Martins Ferreira Batista [1]; Hélio F. Dos Santos [1]; Giovanni Amarante [1]

[1] Universidade Federal de Juiz de Fora

The use of organocatalyst ionic liquid for synthesis of pyranochromene derivates and study of antioxidant and antibacterial activities

https://proceedings.science/p/119557

Jhonathan Santos [1]; Luciana Machado Ramos [1]; Juliana Morais [1]; Yasmine Queiroz [1]; Brenno A. D. Neto [2]
[1] Universidade Estadual de Goiás; [2] Universidade de Brasília

The pyran[3,2-c]chromene compounds were obtained by multicomponent reaction using na ionically marked synthetic enzyme as catalyst. The compounds were sensitive to Staphylococcus aureus (ATCC 29213).

Tissue spray ionization - tandem mass spectrometry (TSI-MS/MS): a new approach for piperamides identification on Piper tuberculatum

https://proceedings.science/p/120417

Aline Garcias de Vargas [1]; João Luiz Bronzel Junior [1]; Maysa Furlan [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

TSI-MS/MS applyed to metabolomic analysis of P. tuberculatum leaves led to the identification of piperamides in an analytical process closer to the green chemistry principles.

Total Synthesis of (+)-Raputindole A via Iridium-catalyzed cyclization.

https://proceedings.science/p/120106

Juliana Lira Luna Freire Regueira [1]; Luiz Fernando da Silva Jr. [1]; Ronaldo Aloise Pilli [2]
[1] Universidade de São Paulo (USP); [2] Universidade Estadual de Campinas (Unicamp)
This work describes the total synthesis of (+)-Raputindole A which features an iridium-catalyzed cyclization, an enzymatic resolution which allows the preparation of enantiomerically pure benzylic alcohol, a methallylation to install the butenyl side chain and a Heck reaction to coupling the northern and southern parts. In our proposal (+)-Raputindole A was prepared in 10 steps (LLS) and 3.3% overall yield.

Tryptophan as target of excited carbonyls: Damage and suppression

https://proceedings.science/p/120428

Luiz Ramos [1]; Camila Marinho Manso [2]; Fernanda Manso Prado [2]; Cassius Stevani [1]; Paolo Di Mascio [2]; Etelvino José Henriques Bechara [1]
[1] Química Fundamental / Instituto de Química / Universidade de São Paulo; [2] Bioquimica / Instituto de Quimica / Universidade São Paulo (USP)

Trp is investigated as a target for excited species
Products arising from the attack of excited and radical species to Trp are identified
Trp might protect biomolecules from damage caused by carbonyl

Unconventional metal-free approach for synthesis of polyfunctionalized fused dihydrobenzimidazoles

https://proceedings.science/p/119491

Michael Jackson Vieira da Silva [1]
[1] Universidade Estadual de Maringá - UEM
TThe polycyclic benzo-imidazo-pyrrolone system is present in chemical entities with very relevant pharmacological properties. One of the most efficient synthetic methods to access this system involve the gold(I)-catalyzed reaction of alkynes bearing tethered carboxylic groups with 1,2-diaminobenzene. However, the high cost is one of drawbacks of this method. In this context, we report here the development of a simple and efficient metal-free synthetic method to access the benzo-imidazo pyrrolone system. The methodology developed is based on the reaction of secondary β-

enamino diketones with o-phenylenediamine through in situ generated of the key intermediate 4-acyl-3,5 dihydroxypyrrolone.

Zinc-Mediated Synthesis of Hydroxy-Ester by Ball Milling Method
https://proceedings.science/p/120277

Thiago Muniz de Souza [1]; Cristiane Kelly de Oliveira [2]; Ivani Malvestiti [3]
[1] Universidade Federal Rural de Pernambuco -UFRPE; [2] Universidade Federal de Pernambuco; [3] Universidade Federal de Pernambuco - UFPE

An efficient and solvent-free synthesis of hydroxy esters by ball milling (mechanochemistry) is developed for zinc-mediated reaction of aromatic and aliphatic aldehydes and ethyl 2-bromopropanoate.

Química Tecnológica - TEC

Analysis of Milk in Natura and Industrialized by TXRF.
https://proceedings.science/p/120224

Amanda Cristina Murari

Chemical elements identified in naturaand industrialized samples were: P, S, Cl, K, Ca, Fe, Zn, Br, Rb e Sr. Differences in the concentrations of chemical elements in both samples.The industrialization process allows changes in concentrations.

Avaliação de N-Acilhidrazonas como Potenciais Quimiossensores Fluorescentes Seletivos a Íons Zn2+
https://proceedings.science/p/119650

Andréa Luzia Ferreira de Souza [1]
[1] UFRJ

Evaluation of N-Acylhydrazones as Potential Fluorescent Chemosensors Selective to Zn2+Ions. The HL2derivative showed a significant fluorescence against the Zn2+ion compared to HL1and HL3derivatives. The fluorescence observed can be related to the inhibition of the PET and isomerization process of the azometine group.

Big Data in Chemical Science applied to penicillin's drugs
https://proceedings.science/p/119672

Jorge Magalhães

Penicillin chemical drugs achieve 1600 patents in last years. Challenges & opportunities in penicillin’s drugs for Brazilian National Health System. Knowledge management in Chemical Big Data Science.

Characterization of silica nanoparticles synthesized by sol-gel method.
https://proceedings.science/p/119811

Vivian Mayumi Shigueoka [1]
[1] Unopar Pitagoras

The silica nanoparticles were synthesized via the Stober method in a basic medium. The characterization of nano-SiO2were carried out by EDXRF (Energy Dispersive X-Ray Fluorescence), AAS (Acoustic Attenuation Spectroscopy) and SEM (Scanning ElectronMicroscopy)

Determination of the biodiesel average molar mass by 1H-NMR with internal standard.

https://proceedings.science/p/120759

Luiz Antonio Mazzini Fontoura [1]; Cristiano de Aguiar Pereira [2]; Samuel Santos [3]; Cassiane Elisabete Mendes Dutra [2]; Dione Silva Corrêa [2]

[1] Universidade Luterana do Brasil; [2] Universidade Luterana do Brasil/Centro de Pesquisa em Produto e Desenvolvimento; [3] Universidade Federal do Rio Grande do Sul

Average molar mass of babassu, canola, lard and soy methyl biodiesels were determined by 1H-NMR.

1,2-dichlorobenzene was used as internal standard for average molar mass determination by 1H-NMR.

Difusão de NaCl e KCl em queijo prato e mussarela no sistema estático e dinâmico.

https://proceedings.science/p/119644

Talita Fogaça de Oliveira Fogaça De [1]

[1] Uel

A difusão multicomponente do NaCl e KCl foi investigada durante o processo de salga de queijo tipo prato e mussarela; A influência dos íons foi analisada em salmoura do tipo estático e dinâmico; A determinação do tempo de equalização foi avaliada por meio da plotagem do perfil das concentrações experimentais e simuladas.

Effectiveness of ozonation for reducing mycotoxins in grains and particulate products

https://proceedings.science/p/120359

Alessandra de Cássia Romero

Decontamination of mycotoxins vary according to molecularstructure. Ozone effectiveness isinversely proportional to particlesize. Permeabilityto ozoneaffects the effectiveness of ozonation

Fixação de pontos quânticos em discos de agarose para a fabricação de dispositivo para análises in situ de águas

https://proceedings.science/p/120403

Renata Soares Teixeira [1]; Mauro Korn [2]; Marco Tadeu Grassi [3]; Maria G. A. Korn [1]; Rodolfo de Melo Magalhães Santana [1]

[1] Universidade Federal da Bahia; [2] Universidade do Estado da Bahia; [3] Universidade Federal do Paraná

Quantum dots fixation strategies were studied aiming their use as luminescent probes for in situ water analysis Quenching of GSH-CdTe@APTES composites was observed for different potential toxic metal

Nanopartículas magnéticas de PHB contendo ftalocianinas metálicas: influência de parâmetros durante o preparo

https://proceedings.science/p/119842

Barbara Silva Figueiredo [1]; André Romero da Silva [2]

[1] Universidade Federal do Espírito Santo; [2] Instituto Federal de Ciência e Tecnologia do Espírito Santo

Photodynamic Therapy (PDT) is a technique that has stood out in the treatment of several diseases, where it involves combining three factors: photosensitizer, light beam and oxygen molecules[1]. As many photosensitizers are lipophilic, it was decided to encapsulate the metallic phthalocyanines (AlPc and InPc), which have great potential for use as a photosensitizer, in polyhydroxybutyrate (PHB) nanoparticles. In order to direct the nanoparticle to the diseased cell, it was decided to encapsulate together with phthalocyanine, iron oxide particles. During the nanoparticles preparation some parameters can influence the properties of the final formulation. For this reason it was decided to investigate the influences of factors such as the metallic atom linked to phthalocyanine - Al (AlPc) and In (InPc) (factor A), the concentration of the polymeric solution - PHB (factor B), the concentration of the stabilizer colloidal - Polyvinyl Alcohol - PVA (factor C) and the agitation speed used (factor D), on the size of the nanoparticles, the entrapment efficiency of the photosensitizers and the recovery efficiency of the PHB nanoparticles, using a factorial design 2^4. The size of the particles was performed by the measurement of the integrate area of the AlPc or InPc-loaded nanoparticle absorbance spectrum (IAAS). The entrapment efficiency was determined using a calibration curve. For this, a mass of lyophilized nanoparticles was dissolved in methylpyrrolidone and the absorbance was measured at the maximum absorbance wavelength. The recovery efficiency was obtained by measuring the mass of the particles after lyophilization. Factor D was the parameter that most influenced the size and efficiency of recovery. The increase in the agitation speed to 20000 rpm caused the IAAS to decrease by 829.07, as well as reduced the recovery efficiency by 12.75%. There is also a significant ternary ACD effect that indicates that the exchange of AlPc during the process of preparing the nanoparticles for InPc, together with the increase in PVA concentration and agitation speed, causes an increase in particle recovery by 9.41%. The exchange of AlPc by InPc during the process of preparing the nanoparticles, also caused the reduction of the photosensitizer entrapment efficiency by 26.34%, being the only significant effect on the photosensitizer encapsulation. Therefore, this work showed that factor D has a great influence on the size of the nanoparticles and their recovery efficiency, reducing both properties, while the exchange of photosensitizer (factor A) decreased the entrapment efficiency.

Síntese de um intermediário de Rosiglitazona em batelada e microrreator capilar

https://proceedings.science/p/120760

Ana Paula dos Santos Cardoso [1]; Paulo Victor Cuesta Calvo [1]; Mauri Palma [1]
[1] Universidade de São Paulo / Faculdade de Ciências Farmacêuticas / Departamento de Tecnologia Bioquímico-Farmacêutica

For the first time, the reaction was transposed to continuous flow, leading to higher yields in shorter times when compared to the batch process, proving that micro reactor is a promising technology.

Química Teórica - TEO

A theoretical study of poly(p-phenylenes) and their cyclodextrin-based insaluted molecular wires

https://proceedings.science/p/120462

Paulo Henrique de Sousa Paulino [1]; Luciana Guimarães [1]; Clebio Soares Nascimento Jr. [2]
[1] Departamento de Ciências Naturais / Campus Dom Bosco / Universidade Federal de São João del-Rei; [2] Universidade Federal de São João del-Rei

*HOMO-LUMO gaps were obtained before and after the encapsulation process of the PPP oligomers into the β-CD tubes.
*The conductive properties of PPPs are maintained when they are covered by CDs.

Abordagem computacional para avaliar a enantiosseletividade na síntese de 2-Aril-2,3-diidro-4-quinolonas por meio de organocatálise

https://proceedings.science/p/120585

Patrick de Lima Rocha [1]; Rodolfo Goetze Fiorot [2]; Sérgio Pinheiro [3]
[1] MEC (Ministério da Educação) - Universidade Federal Fluminense; [2] Universidade Federal Fluminense; [3] Universidade Federal Fluminense, Departamento de Química Orgânica

Syn and anti Zimmerman-Traxler “chair-like” diastereoisomeric transition states are located with DFT methods. A 55% of ee% is estimated, in excellent agreement with experimental results (59%).

AC/DC analysis: a theoretical protocol to evaluate IR intensities at the atomic level

https://proceedings.science/p/119752

Wagner Richter [1]
[1] Universidade Tecnológica Federal do Paraná

The outer hydrogen stretches in the HNgX dimers are probably the strongest IR bands ever calculated; Further analyses through the QTAIM/CCTDP model show terms even stronger than the total intensity itself;

Adsorption of [Fe(OH)x(H2O)y]z species on the (001) and (112) chalcopyrite surface x0096 A DFT study

https://proceedings.science/p/120262

Selma Fabiana Bazan [1]; Guilherme de Lima [1]; Helio Anderson Duarte [1]
[1] Universidade Federal de Minas Gerais

- (001) and (112) Chalcopyrite surfaces models; - Adsorption of [Fe(OH)x(H2O)y]3-x; - DFT.

An Interacting Quantum Atoms (IQA) Approach to the Reverse Lewis Acidity of Boron Trihalides.

https://proceedings.science/p/120061

Leonardo Duarte [1]; Wagner Richter [2]; Roy Edward Bruns [1]; Paul Popelier [3]
[1] UNICAMP; [2] UTFPR; [3] University of Manchester

The reaction path for the formation of the BX3-NH3 (X = H, F, Cl, Br) complexes, was divided into two major processes: 1 – rehybridization of the acid, adopting a pyramidal geometry, and; 2 – complex formation from the pyramidal geometries of the acid and base. An Interacting Quantum Atoms approach was applied to investigate the Lewis acidity trend presented by these compounds. Topological analysis suggests that the boron-halogen bond exhibits a considerable degree of ionicity. Relative Gradient Analysis associated with the IQA partition indicates the acid-base complex formation is highly dependent on classical electrostatic potential. With the increase of X electronegativity, a higher degree of ionicity of the B-X is observed, causing an increase in the absolute value of X and B charges, increasing not only the attractive potentials between acid and base, but the repulsive potentials are also enhanced. This increase in the repulsive potentials is the main factor behind the acidity trend exhibited by the trihalides. Changes in geometry are relevant only for complexes where BH3 acts as an acid, where lower steric hindrance facilitates the adoption of the pyramidal geometry observed in the complex. The CCTDP analysis shows that infrared intensities of BX3-NH3 are determined mostly by the atomic charges, and not by the charge transfer or polarization. The opposite is observed in covalent analogs.

Chemical Bonds Overlap Properties and Dissociation Pattern in CH5+

https://proceedings.science/p/120625

Francielle Carolinne Machado Santos [1]; Renaldo Moura Jr [1]
[1] Universidade Federal da Paraíba – Campus Areia

Overlap properties calculated for CH5+ corroborate the pattern CH3 ⋯ H2+ CH3+ ⋯ H2 upon dissociation, also indicated by valence bond calculations. QTAIM do not follow this same trend.

COMPUTATIONAL STUDY OF FIRST HYPERPOLARIZABILITY OF RUTHENIUM COMPLEXES WITH POTENTIAL TECHNOLOGICAL APPLICATION

https://proceedings.science/p/120430

Júlio de Paula Campbell Oliveira [1]; Diego Fernando da Silva Paschoal [1]; Hélio F. Dos Santos [2]
[1] Universidade Federal do Rio de Janeiro; [2] Universidade Federal de Juiz de Fora

We evaluate the influence of level of theory and basis sets for metal/ligands in predicting first hyperpolarizability of ruthenium complexes with potential technological application.

Desenvolvimento de rotinas computacionais para cálculos de espectros vibronicos a partir de trajetórias clássicas e a distribuição de Wigner

https://proceedings.science/p/120400

Bárbara Júlia Gonçalves Dutra [1]; Freddy Fernandes Guimarães [1]
[1] Universidade Federal de Goiás

Computation of the HCl vibronic spectrum at the X-ray energy region.

DFT analysis of organocatalysis with NHCs and alcohols co-initiators in poly(lactones) formation

https://proceedings.science/p/120557

José Renato Duarte Fajardo [1]; Milena Diniz Lessa [1]; José Walkimar de Mesquita Carneiro [1]
[1] Universidade Federal Fluminense

The formation of poly(lactones) has as main process the Ring Opening Polymerization. NHCs can potentially act as a nucleophile (attack on the monomer, zwitterion) or base (attack on the co-initiator).

Enantioselective Separation of Atenolol: A Theoretical Study

https://proceedings.science/p/120469

Pollyanna Pinto Maia [1]; Clebio Soares Nascimento Jr. [2]; Lilian Christina Zin [3]
[1] Universidade Federal de São João del Rei; [2] Universidade Federal de São João del-Rei; [3] Departamento de Ciências Naturais / Campus Dom Bosco / Universidade Federal de São João del-Rei

Theoretical investigation of the enantioselective separation mechanism of atenolol using carboxymethyl-β-Cyclodextrin as chiral selector;
The migration order of the atenolol enantiomers was elucidated

Estudo computacional sobre a formação de oximas pela oxidação de aminas por m-CPBA

https://proceedings.science/p/120012

Ana Carolina Moralles Barbosa Silva [1]; Fabrício Ronil Sensato [2]
[1] Universidade de Campinas, Instituto de Química; [2] Universidade Federal de São Paulo, Instituto de Ciências Ambientais, Químicas e Farmacêuticas

The study reveals that in OAT steps, an interaction between the peroxy acid σ*(O—O) level and the amine HOMO occurs. A linear correlation is found between the ΔG‡ and the peroxy acid σ*(O—O) level.

Estudo da redução eletroquímica do corante Disperse Violet 93 via Modelagem Molecular

https://proceedings.science/p/120437

Júlia Paiva Copola [1]; Julliane Yoneda Huguenin [1]; Patrícia Alves Carneiro [1]
[1] Universidade Federal Fluminense

Applying Molecular Modeling to study the electrochemical degradation in acidic medium of Disperse Violet 93 dye.

Modeling the inclusion complexes of cisplatin and its aquated species with functionalized carbon nanohorns: a quantum chemical approach

https://proceedings.science/p/120427

Eduardo Ribeiro Almeida [1]; Wagner Batista de Almeida [2]; Jadson Claudio Belchior [3]; Leonardo Aparecido de Souza [3]; Hélio F. Dos Santos [1]
[1] Departamento de Química, Universidade Federal de Juiz de Fora; [2] Departamento de Química Inorgânica, Universidade Federal Fluminense; [3] Departamento de Química, Universidade Federal de Minas Gerais

Carbon nanohorns (CNH) are potential nanovectors of cisplatin (cddp). Chemical functionalization can improve the biocompatibility of these materials. The cddp hydrolysis can take place inside the CNH.

Organocatalyzed Nitro-Michael Addition Reaction: Theoretical Free Energy Profile and Benchmarking of Functionals

https://proceedings.science/p/119970

Josefredo Rodriguez Pliego Júnior [1]
[1] UFSJ

QSARModelingPy: a python package to build and validate QSAR models.

https://proceedings.science/p/120640

Joao Paulo Ataide Martins [1]; Héliton Martins Reis Filho [1]
[1] Universidade Federal de Minas Gerais

QSARModelingPy evolves from *QSAR Modeling* (MARTINS; FERREIRA, 2013), a software focused on the build and validation of QSAR and QSPR models. Developed in Python 3, this new version comes to solve some problems present in the previous version, written in Java 6. For example, the old version was black box, what indicates a lower suitability and scalability of the software, as well limits its execution to a local machine. To solve that, the Python version has multiple interfaces and is open-source. Because it has a Graphical User Interface, a Jupyter Notebook implementation, a headless command line version and a library hosted on the Python Package Index (PyPI), its use is facilitated from the end user with no programming knowledge to a fully programmatic or remote environment. In addition, some features have also been included such as the external validation and variable selection using Genetic Algorithm, which generally shows better results than the selection done with the Ordered Predictors Selection (OPS) algorithm. 2D and 4D-QSAR models were built with this program using the Genetic Algorithm for two data sets of synthetic tetronamides displaying inhibitory activity against the photosynthetic electron transport chain in isolated spinach chloroplasts and the photoautotrophic growth of the model cyanobacterium *S. elongatus* (ACOSTA *et al*, 2019). The obtained Q^2 values for the first assay were 0.79 (2D) and 0.75 (4D). For the latter, these values were 0.72 (2D) and 0.89 (4D).

Quantum chemical studies of the reactivity and NMR spectroscopic properties on new piperine derivatives

https://proceedings.science/p/120461

Evandro Paulo Soares Martins [1]; Helivaldo Souza [2]; Joselito Júnior [2]; Petrônio Athayde Filho [2]; Gerd Rocha [2]
[1] Universidade Estadual do Piauí; [2] Universidade Federal da Paraíba

New piperine derivatives were synhesized
DFT studies of the compounds were carried out

Reconhecimento quiral de drogas β-bloqueadores por colunas de cromatografia de polissacarídeos substituídos: um estudo computacional

https://proceedings.science/p/120454

Camilla Fonseca Silva [1]; Pollyanna Pinto Maia [2]; Camila de Araujo Nascimento [3]; Clebio Soares Nascimento Jr. [1]
[1] Universidade Federal de São João del-Rei; [2] Universidade Federal de São João del Rei; [3] Universidade Federal do Oeste do Pará

Theoretical study of the chiral recognition mechanism of β-blockers, atenolol (ATL) and carvedilol (CVL) by Density Functional Theory (DFT) calculations.

Structural and spectroscopic studies of chloroacetone and its molecular ion

https://proceedings.science/p/119695

Diego de Oliveira Rogério [1]; Alexsandre Figueiredo Lago [2]
[1] Universidade Federal do ABC; [2] Universidade Federal do ABC (UFABC)

A theoretical study on the structures of the chloroacetone molecule and cation has been performed. Properties, such as IR spectra and ionization potential are in good agreement with experimental data.

Studies of BaZrO3 first structural and electronic principles

https://proceedings.science/p/120616

Suellen Matias Ferreira [1]; Nélio Henrique Nicoleti [1]
[1] IFSP

This study aims to perform a computational modeling of BaZrO3, to obtain a model that approximates the experimental results regarding the material's properties and electronics.

The ternary hydrogen-bonded complexes formed by pseudo-π···H and N···H interactions: DFT and QTAIM calculations

https://proceedings.science/p/119817

Daniel Arley Santos Oliveira [1]; Boaz Galdino Oliveira [1]; Danilo Guimarães do Rego [1]
[1] Universidade Federal do Oeste da Bahia

This work consists of a theoretical study of ternary complexes stabilized through the hydrogen bonds. Analyses of structural and topological parameters were carried out.

The Trans Effect in Platinum (II) Complexes: An Analysis from the Overlap Model.

https://proceedings.science/p/120125

Gabriel Augusto Lyra Porto [1]; Thiago Emanuel Monteiro de Oliveira [1]; Vinícius Nascimento [2]; Roberta P. Dias [3]; Renaldo Moura Jr [2]; Júlio Cosme Santos da Silva [1]
[1] Universidade Federal de Alagoas; [2] Universidade Federal da Paraíba; [3] Universidade Federal de Pernambuco
Full DFT mechanistic characterization of the substitution reaction in square-planar Pt(II) complexes in solution as well the chemical nature of M-T(ligand) and M-H2O interactions via overlap model.

Theoretical Investigation of the Mechanism of Acid-catalyzed Dehydration of Pyrazol-4-ol in Methanol Solution

https://proceedings.science/p/119534

Edna Carolina Cipagauta Esquivel [1]; Virgínia Camila Rufino [1]; Matheus Henrique Trindade Nogueira [1]; Ana Carolina Carbonaro Souza [1]; Josefredo Rodriguez Pliego Júnior [1]; Marcelo Siqueira Valle [1]
[1] UFSJ

The synthesis of diverse pyrazol-4-ol and isoxazole-4-ol heterocycles involving only 3 reaction steps is reported in this study. However, the synthesis of carboxamide pyrazol-4-ol has failed in the conditions used in the synthesis, acid methanol solution. The carboxamide pyrazol-4-ol decomposes via dehydration, forming the respective pyrazol. Theoretical calculations were used to elucidate the dehydration reaction. We have found a mechanism for acid-catalyzed dehydration that can explain the experimental observations. The calculated free energy profile for acid-catalyzed dehydration of the carboxamide pyrazol-4-ol and phenylpyrazole-4-ol point out that the latter is more stable in relation dehydration, with a dehydration rate 100 times smaller in acid methanol solution.

Theoretical study of the cooperative effect of solvent in the mechanism for the Markovnikov addition of HCl to 1-Butene

https://proceedings.science/p/120510

Nelson Henrique Morgon [1]; Caio Moraes Porto [2]; Lucas Chuman Santana [3]
[1] UNICAMP; [2] Universidade Estadual de Campinas - Instituto de Química; [3] Universidade Estadual de Campinas

* Solvent effects were investigated via implicit and hybrid explicit/implicit treatments
* The hybrid solvent model improved the efficiency of simulations
* Electronic Circular Dichroism spectra

Química Verde - QVE

Água como solvente na síntese de novos derivados de isatina: uma metodologia de Química Verde

https://proceedings.science/p/120624

Mayara dos Santos Baptista [1]; Thaisa Ribeiro Henriques Quinteiro [1]; Mariana Carvalho Oliveira [1]; Vinicius Campos [1]; Anna Cláudia Cunha [1]
[1] Universidade Federal Fluminense

This work describes the planning and synthesis of 6 phenilhydrazonic derivatives of isatin, replacing the use of harmful solvents with water based on some principles of green chemistry.

Biodiesel de óleo de soja produzido a partir de grãos de soja com diferentes teores de água

https://proceedings.science/p/119833

Daniela Reolon [1]; Caroline Cassalha Schneid [1]; Renata Zachi de Osti [1]; Gustavo Giraldi Shimamoto [2]; Matthieu Tubino [2]; Eva Lúcia Cardoso Silveira [1]
[1] Universidade Federal de Mato Grosso - Câmpus Sinop; [2] Universidade Estadual de Campinas

The production of biodiesel from oils obtained from grains with high content of water can contribute to the reduction of the biofuel cost with respect to the use of dried grains.

Determinação do método rápido e verde de minerais em soja usando espectroscopia infravermelha (NIRS)

https://proceedings.science/p/120587

Suzana Caetano Rodrigues Gonçalves [1]; Francisco Panero [1]; João dos Santos Panero [1]; Pedro dos Santos Panero [2]; Fernando Sérgio Escócio Drummond Viana de Faria [3]; Anselmo Fortunato Ruiz Rodriguez [3]
[1] Universidade Federal de Roraima; [2] Instituto Federal de Ciências e Tecnologia de Roraima; [3] Universidade Federal do Acre

spectroscopy combined with multivariate analysis: Partial Least Squares
(PLS) for rapid and non-destructive determination (prediction) the levels (mg.Kg-1) Ca, K, Mg, Fe, Zn, P and Sr

DISCRIMINAÇÃO DE CULTIVARES DE GERGELIM ATRAVÉS DA ESPECTROSCOPIA NIR E QUIMIOMETRIA

https://proceedings.science/p/119587

Bárbara Victória Grigório Barbosa [1]; Francisco S. Panero [1]; João Panero [2]; Anselmo F. R. Rodriguez [3]; Cristofe C. L. da Rocha [2]; Pedro dos Santos Panero [2]; Fernando S. E. D. V. Faria [3]
[1] Universidade Federal de Roraima; [2] Instituto Federal de Roraima; [3] Universidade Federal do Acre

Este trabalho investiga o potencial da espectroscopia NIR combinada com análise multivariada: PCA e HCA para autenticação forense rápida e não destrutiva de grãos de arroz do Brasil e da Venezuela.

Effect of epoxidation and maleinization reactions on grape seed oil thermal properties and on its viscosity

https://proceedings.science/p/120556

Caroline Gaglieri [1]; Rafael Turra Alarcon [1]; Raquel Magri Magri [1]; Luiz Carlos da Silva-Filho [1]; Gilbert Bannach [1]
[1] Universidade Estadual Paulista "Júlio de Mesquita Filho"

Grape seed oil (GSO) is a wine and juice by-product with high application potential. GSO can be modified by clean and fast synthesis.

Electrooxidation of organic substances in heterogeneous phase following some of the principles of Green Chemistry

https://proceedings.science/p/120509

Claudemir Batalini [1]; Wagner Ferraresi de Giovani [1]
[1] Universidade Federal de Mato Grosso - Campus Universitário do Araguaia, Pontal do Araguaia (MT)

Electrooxidations of organic functions in a heterogeneous phase were carried out in a process less aggressive to the environment.

EVALUATION OF BIOKEROSENE PRODUCTION FROM COTTONSEED OIL DREG BY CATALYTIC MICROPYROLYSIS

https://proceedings.science/p/119670

Mirele Santana de Sá [1]; Josué Alves Melo [2]; Jhonattas Carregosa [1]; Fernando Bimbela Serrano [3]; Luis Maria Gandia Pascual [3]; Ainara Moral Larrasoana [3]; Alberto Wisniewski Jr [1]
[1] Universidade Federal de Sergipe, Brasil.; [2] Federal University of Sergipe; [3] Public University of Navarra, Spain.

Total conversion of carboxylic acids using Mo-Co/α-Al2O3 as catalyzer.
Production of bio-oil from cottonseed oil residue composed by 97.5% of compounds in kerosene range, via catalytic hydropyrolysis.

INFLUENCE OF PYROLYSIS REACTORS DESIGN UPON CHEMICAL COMPOSITION OF CATTLE MANURE BIO-OIL

https://proceedings.science/p/119721

Tarcisio Martins Santos [1]; Wenes Ramos da Silva [2]; Jhonattas Carregosa [1]; Alberto Wisniewski Jr [3]
[1] Universidade Federal de Sergipe; [2] Universidade Federal de Sergipe - UFS; [3] Universidade Federal de Sergipe, Brasil.

Chemical characterization at molecular level of polar fraction from Cattle manure bio-oil using FT-Orbitrap MS; Renewable fine chemicals to substitution of fossil-type products in petroleum industry.

Microwave-assisted ethyl levulinate production from water-soluble sugars and sugarcane molasses mediated by taurine hydrogen sulfate

https://proceedings.science/p/120207

Gustavo Rodrigues Gomes [1]; Julio Cezar Pastre [1]
[1] Universidade Estadual de Campinas (UNICAMP)

Plasticizing effect of different Deep Eutectic Solvents on the transparency property of starch-based biofilms.

https://proceedings.science/p/120292

Rachel Azevedo Maia [1]; Isadora Maria Gouveia Andrade [2]; Priscila Micaelly da Silva Costa [2]; Francisco de Assys Romero de Mota Sousa [1]; Silvanda Silva [1]; Dayse das Neves Moreira [1]
[1] Universidade Federal da Paraíba; [2] Universidade Federal da Paraíba – Campus Areia

Starch-based films have gained attention due to the possibility of replacing, even if partially, synthetic polymers, which are responsible for several ecological problems.1 Due to strong interactions between starch chains, it is necessary the use of plasticizing to create more flexible materials.2 In this context, glycerol has been the most used plasticizer in the production of those films, but because of its high hygroscopicity it can lead to starch retrogradation after a long time of storage.3 Recently, Deep Eutectic Solvents (DES), which are mixtures of two or more compounds that present a mixture melting point lower than that of any individual component, have been evaluated as a likely plasticizer. Thus, some DES based on choline chloride with glycerol and urea, carboxylic acids and imidazole have already been demonstrated as good starch plasticizers.4 In this work, we studied the influence of three different DES (ChCl:Cit 1:1; Pro:Cit 1:2 and Bet:Cit 1:1) as plasticizing agents for the starch-based biofilms formulation. DES were prepared by stirring the components at 80 °C, for 2 h. The films were prepared following the casting method, which consists of heating a 3% aqueous solution of starch. Table 1 shows the DES synthesized herein, the molar ratio used, and the biofilms characterization data (thickness was measured using a digital micrometer, and transparency, a UV-Vis spectrometer). From the data obtained, we observed that the DES-based films were significatively thinner than the glycerol pattern. In addition, DES ChCl:Cit achieved the best results in terms of transparency, being more than twice greater of the film with Gly.

Rapid and Green method determination of acetaminophen by Herschel-infared reflectance

https://proceedings.science/p/119542

Francisco Panero [1]; Rosana Ferreira de Sousa [2]; Pedro dos Santos Panero [3]; Henrique Eduardo Bezerra da Silva [4]; João Panero [5]; Jarbas Rohwedder [6]
[1] Universidade Federal de Roraima; [2] UFRR; [3] Instituto Federal de Ciências e Tecnologia de Roraima; [4] Universidade Federal do Rio Grande do Norte; [5] IFRR; [6] Universidade Estadual de Campinas

Rapid and Green method determination of acetaminophen by Herschel-infared reflectance

Rapid and Green method forensic authentication of rice using near-infrared spectroscopy (NIRS) and multivariate analysis

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Francisco Rony Barreto Alves [1]; Francisco Santos Panero [1]; João Santos Panero [2]; Pedro Santos Panero [2]; Anselmo F. R Rodriguez. [3]; Fernando S. E. D. V. Faria [3]

[1] UFRR; [2] IFRR; [3] UFAC

Rapid and Green method forensic authentication of rice using near-infrared spectroscopy (NIRS) and multivariate analysis Francisco S. Panero (PQ),1* Francisco R. B. Alves (IC),1 João S. Panero (PQ),2 Anselmo F. R. Rodriguez (PQ),3 Pedro S. Panero (PQ),2 Fernando S. E. D. V. Faria (PQ).3 thebicus@gmail.com; francisco.panero@ufrr.br 1Chemistry Department, Federal University of Roraima, UFRR 2Federal Institute of Science and Technology of Roraima, IFRR; [3]Biodiversity and Biotechnology Network of the Legal Amazon, Biotechnology Department, Federal University of Acre, UFAC Keywords: Near-Infrared, Rice, Chemometrics, forensic authentication. Highlights Rapid and Green method forensic authentication of rice using near-infrared spectroscopy (NIRS) and multivariate analysis This work investigates the potential of NIR spectroscopy combined with multivariate analysis: PCA and HCA for rapid and non-destructive forensic authentication of rice grains from Brazil and Venezuela. Abstract Nowadays, scientists are seeking to develop methodologies that do not harm the environment. In the literature, some researchers have proposed the new concept of "Green Chemistry", which is sometimes called "Clean Chemistry" or "Environmentally Benign Chemistry". Green Chemistry refers to the use of a set of principles that prioritize the reduction or elimination of the use or generation of hazardous substances in the design, manufacture, and application of chemicals. Anastas and Warner1 proposed 12 complementary principles in order to maximize resource efficiency and minimize the environmental and human health risks. The most important of the twelve principles is the first (because avoiding waste is better than treating or cleaning the waste generated). Many conventional analytical methods are not green, as they produce harmful residues during and after analytical processes. However, the key priorities4 can reduce or eliminate reagent consumption and minimize the working time through highly efficient analyses. The analytical methods used in green chemistry are an important trend in analytical chemistry because of sustainable development that is useful for society. Authenticity is an important issue for the food industries due to legal compliance, economic reasons and guarantee of quality. But the majority of analytical methods and techniques used for authentication and discrimination of geographical origin of food products are destructive, slow and generate waste to the environment. Considering rice as a raw material of economic and social value and the recent use of NIR spectroscopy coupled with chemometric methods to authentication and discrimination of geographical origin as an alternative to classical methods in the search for a methodology in line with Green Chemistry, this work investigates the potential of NIR spectroscopy combined with multivariate analysis: PCA (Principal Component Analysis) and HCA (Hierarchical Cluster Analysis) for rapid and non-destructive forensic authentication of rice grains from Brazil and Venezuela. For this study two commercial rice (Faccio and Prato Chic) produced in the State of Roraima (Brazil) acquired in the local commerce and a one commercial rice (Cristal) originating in Venezuela obtained in the informal free fairs where products from the neighboring country (Venezuela are found). This study investigated the potential of near infrared spectroscopy, combined with PCA and HCA chemometric technique to authenticity of Rice. is feasible and advantageous to implement authenticity detection authenticity of different brands, typology and geographical discrimination (Brazil and Venezuela) rice. It can serve as an alternative to laborious, time-consuming, wet chemical methods and sensory analysis of human. References [1]P. T. Anastas and J. C. Warner, Green Chemistry: Theory and Practice, Oxford University Press: New York, 1998. [2]American Chemical Society. https://www.acs.org/content acs/en/greenchemistry/what-is-green-chemistry/principles/ 12-principles of-green-chemistry.html (accessed December 2019)

Synthesis and characterization of high surface area biocarbon derived from sugar and alcohol industry wastes.

https://proceedings.science/p/120039

Eduardo Emanoel Batista [1]; Lenivaldo V. Sousa [2]; Aracelis José Pamphile Adrian [2]; Pedro Pablo Florez Rodriguez [2]

[1] Universidade Federal de Alagoas ; [2] Universidade Federal de Alagoas

Synthesis and characterization of high surface area biocarbon, derived from sugar and alcohol industry wastes. Different granulometric fractions were found. Organic and inorganic matter were identified, with Si as main inorganic component. A surface area of 480 m2 /g was obtained.

The influence of Deep Eutectic Solvents in the production of corn starch-based biofilms

https://proceedings.science/p/120263

Isadora Maria Gouveia Andrade [1]; Rachel Azevedo Maia [2]; Priscila Micaelly da Silva Costa [1]; Silvanda Silva [2]; Dayse das Neves Moreira [2]

[1] Universidade Federal da Paraíba – Campus Areia; [2] Universidade Federal da Paraíba

The effect of deep eutectic solvents has been studied. Plasticizer agent. Biofilms that are more resistant to storage. Development of more efficient methodologies for polymer production.

USY-zeolite catalyzed synthesis of 1,4-dihydropyridines under microwave irradiation: structure and recycling of the catalyst

https://proceedings.science/p/120514

Leonardo Henrique Rondina Alponti [1]; Arlene Corrêa [1]; Monize Picinini [1]; Ernesto Antonio Urquieta-González [1]

[1] Universidade Federal de São Carlos

Multicomponent reactions, use as a green processes, allow the synthesis of molecules in one-pot way. The dihydropyridine had potent biological activities. The USY zeolite had good catalytic behavior.