

química nova

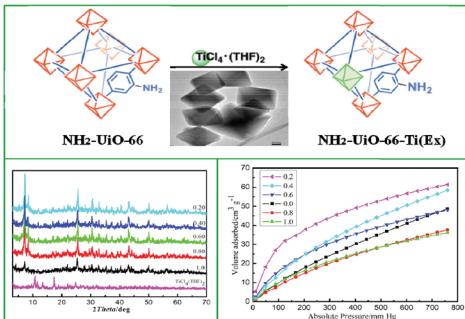
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Artigo

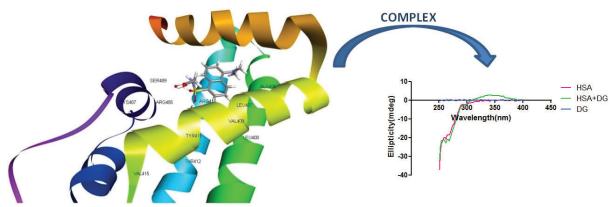
- 129 Postsynthesis of Titanium incorporated with amino-functionalization UiO-66 for enhancing CO₂ uptake
Jinlong Ge, Zhong Wu, Qiuqin Wang and Shanshan Yang



Titanium cooperated with $\text{NH}_2\text{-UiO-66}$ has been prepared via post synthesis modifications approach and perform enhanced CO_2 uptake application due to their unprecedented capacity to store small molecules.

- 135 Elucidação da quiralidade induzida na molécula dansilglicina na complexação com a proteína albumina do soro humano (HSA)

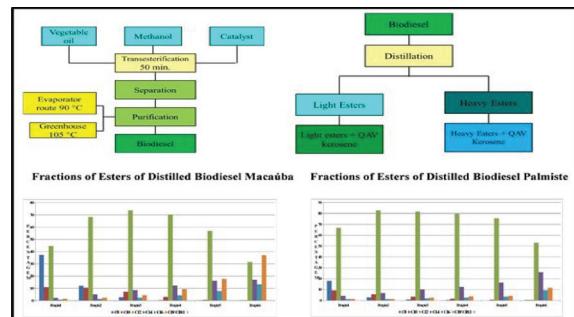
Aguinaldo R. de Souza, Izabelle A. F. Boza, Valdecir F. Ximenes, Maurício I. Yoguiun, María-José Dávila-Rodríguez, Nelson H. Morgen e Ignez Caracelli



An induced circular dichroism (ICD) signal is obtained by complexation between human serum albumin (HSA) and dansylglycine (DanG).

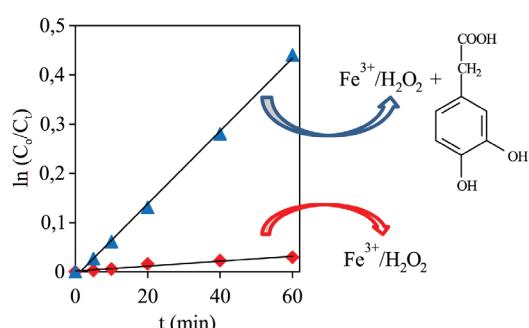
- 143 Destilação atmosférica do biodiesel derivado do óleo de macaúba ou do palmiste para obtenção da fração de ésteres leves para uso como combustível de aviação

Luiz V. L. Harter, Douglas Q. Santos e José D. Fabris



- 149 Um estudo cinético sobre a influência de mediadores fenólicos na descoloração de diferentes corantes por sistemas Fenton

Cássia S. Santana, Camila C. V. Velloso e André Aguiar

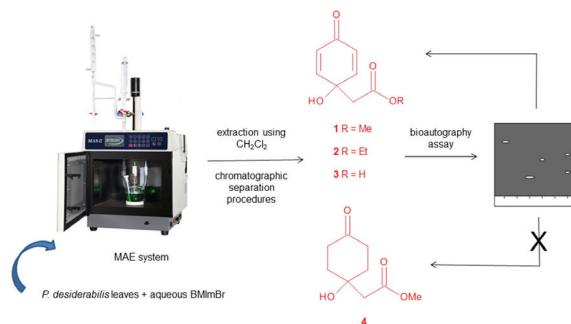


The presence of the phenolic mediator, 3,4-dihydroxyphenylacetic acid, increased the reaction rate to the phenol red decolorization by a Fenton system.

- 156 Isolation of antifungal quinoid derivatives from leaves of *Pentacalia desiderabilis* (Vell.) Cuatre. (Asteraceae) using ionic liquid in the microwave assisted extraction

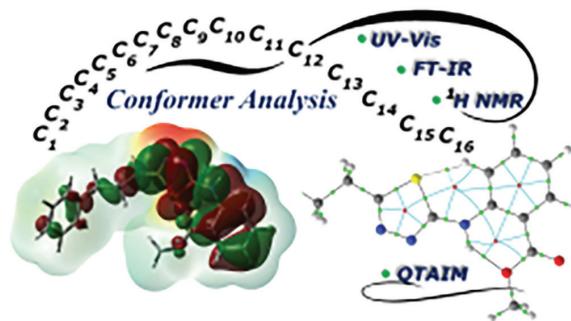
Kaio de S. Gomes, Cinthia I. Tamayose, Marcelo J. P. Ferreira, Cynthia Murakami, M^a Claudia M. Young, Guilherme M. Antar, Fernanda F. Camilo, Patricia Sartorelli and João H. G. Lago

Leaves of *Pentacalia desiderabilis* (Asteraceae) were extracted using BMImBr and H₂O in a MAE system. Partition with CH₂Cl₂ and fractionation of organic phase afforded four related quinoids (1 - 4). Compounds 1 - 3 displayed activity against *Cladosporium* sp.



- 159 Synthesis, electronic and spectral properties of new 1,3,4-thiadiazole compounds and the spectral analysis of their conformers using density functional theory

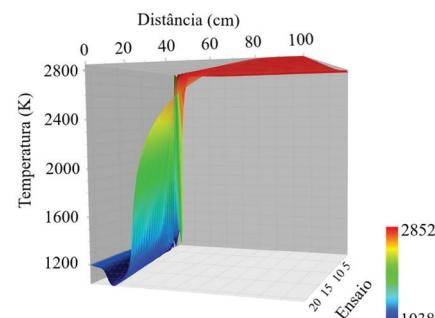
Muhammet S. Çavuş and Tuğba Çelik



Analysis of the correlation between electronic and spectral data of the conformers of new 1,3,4-thiadiazole compounds.

- 173 Simulação de combustão do polibutadieno líquido hidroxilado, perclorato de amônio e alumínio em formulações de propelente sólido compósito

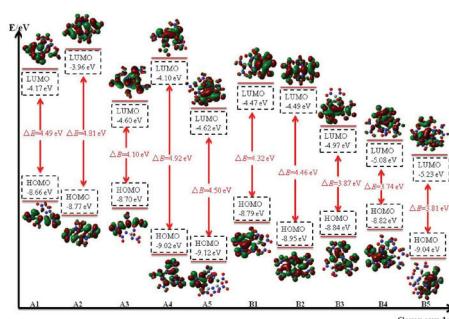
Renata F. Cardoso, Luciene D. Villar, Elizabete Y. Kawachi e Rene F. B. Gonçalves



Influence of the axial velocity on the initial temperature developed during the propellant burning process.

- 181 Molecule design and properties of cyclic energetic materials based on nitroguanidine and 1,1-diamino-2,2-dinitroethene

Xiao Menghui, Jin Xinghui, Zhou Jianhua and Hu Bingcheng

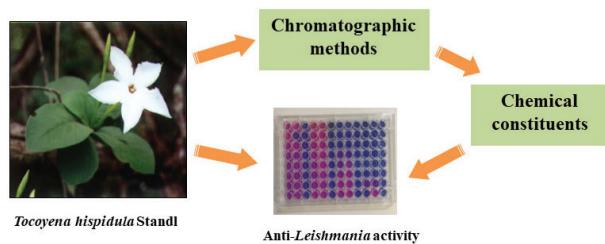


A series of nitroguanidine and 1,1-diamino-2,2-dinitroethene based cyclic energetic materials were designed and their electronic structures, detonation properties and thermal stabilities were fully investigate by density functional theory (DFT).

192 Composição química e atividade antileishmania de *Tocoyena hispidula*

Elcilene A. de Sousa, Amauri Porto A. Rosa, Rodolfo R. L. dos Santos, Ingredy L. dos Santos, Valéria C. de Sousa, Fernando A. de A. Carvalho, Gerardo M. Vieira Júnior e Mariana H. Chaves

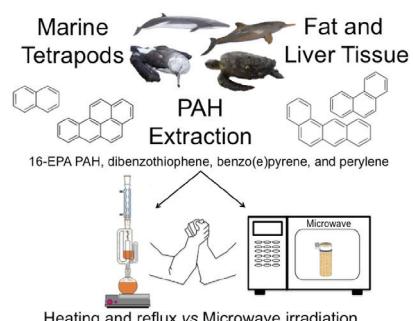
Phytochemical study of the CHCl₃ fraction from EtOH extract of *T. hispidula* stem led to the isolation of six pure compounds and four mixtures, predominantly triterpenoids and steroids. The CHCl₃ and EtOAc fractions were the most active against *Leishmania major* promastigotes.



197 Comparação entre técnicas de extração de hidrocarbonetos policíclicos aromáticos em tecidos hepático e adiposo de tetrápodes marinhos e avaliação da heterogeneidade dos tecidos

Rafael A. Lourenço, Satie Taniguchi, Josilene da Silva, Patrick S. Dias e Márcia C. Bícego

Comparison between two PAH extraction techniques, soxhlet and microwave irradiation, in biological tissues of marine tetrapods. Validation of analytical methods and procedures.

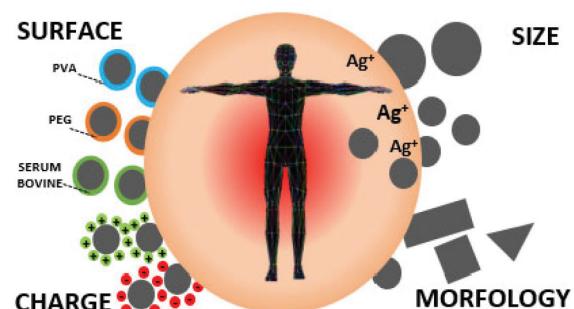


Revisão

206 Nanotoxicologia de nanopartículas de prata: toxicidade em animais e humanos

Nelson Durán, Wallace R. Rolim, Marcela Durán, Wagner J. Fávaro e Amedea B. Seabra

This review presents a critical view of the toxic effects of silver nanoparticles (Ag NPs) on *in vitro* and *in vivo* biological models.

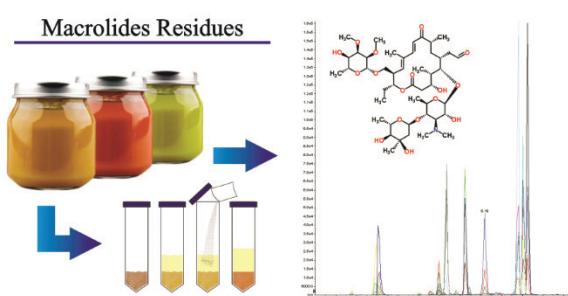


Nota Técnica

214 Avaliação de diferentes métodos de extração para a identificação de resíduos de macrolídeos em alimentos infantis industrializados à base de carne por cromatografia a líquido acoplada à espectrometria de massas sequencial (LC-MS/MS)

Jônatas V. Grutes, Rosana G. Ferreira, Mychelle A. Monteiro, Mararlene U. Pereira e Bernardete F. Spisso

This study compared eight simple methods for identification of macrolides residues in canned baby food and an effective extraction method was achieved, using QuEChERS procedure for sample preparation.



Educação

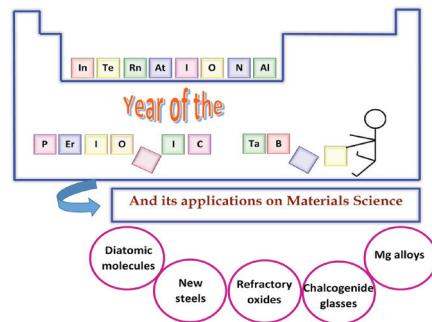
- 221 Exposição Oral no Ensino Superior de Química
Patrícia F. de O. Cabral, Keila A. Peron e Salete L. Queiroz



Using the topic of biodiesel as a platform, we have created a series of activities designed to provide undergraduate chemistry students the opportunity to develop oral communication skills.

- 232 La periodicidad de los elementos y el desempeño de los materiales: un complemento para la comprensión de la tabla periódica

Virginia E. Noval y José G. Carriazo

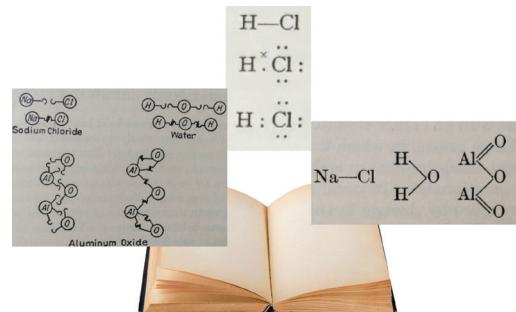


The United Nations has proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements. For that reason, it is considered pertinent to highlight the importance of the periodic system in the scientific and technological development of the chemistry.

Assuntos Gerais

- 237 O conceito de valência em livros didáticos de Química Geral entre as décadas de 1890 e 1940

Helena S. A. Nogueira e Paulo A. Porto



In the first decades of the 20th century, general chemistry textbooks presented the concept of valence in different ways, from classical approaches to the electronic model. Didactic models might include even an analogy with hooks holding atoms together.