ISSN 0103-5053

Journal of the Brazilian Chemical Society

Vol. 29, No. 4, April, 2018

Cover Picture



The present study evaluated the inhibitory activity of new eugenol esters on *Leishmania* rCPB 2.8 enzyme aiming to discover new promising drug candidates. Activation and enhancement of the *in vitro* proteolytic activity of this enzyme were also produced by some compounds and may be related to their preference in binding to an allosteric site, possibly located in the region of the LYS159 residue, close to the active site. Details are presented in the Article **Design, Synthesis, Biological Evaluation and Molecular Modeling Studies of Novel Eugenol Esters as Leishmanicidal Agents** by *Camila M. Coelho, Thiago dos Santos, Poliany G. Freitas, Juliana B. Nunes, Marcos J. Marques, Camila G. D. Padovani, Wagner A. S. Júdice, Ihosvany Camps, Nelson J. F. da Silveira, Diogo T. Carvalho and Marcia P. Veloso on page 715.*

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680 **Oualitative and Ouantitative Chemical Investigation** of Orthopedic Alloys by Combining Wet Digestion, Spectroanalytical Methods and Direct Solid Analysis Caio M. Figueiredo, Jeyne P. Castro, Marco A. Sperança, Lucimar L. Fialho, Joaquim A. Nóbrega and Edenir R. Pereira-Filho

Graphical Abstract

Laser-based analytical techniques for direct qualitative evaluation of orthopedic Ti alloys, and results comparison with data obtained after microwave-assisted digestion and inductively coupled plasma optical emission (ICP OES) determination.

689 **Electrocatalytic Oxidation Removal of Phenol from Aqueous** Solution with Metal Oxides Doped Carbon Aerogel Gui-Fen Lv, Yuan-Hua Chen, Tao Yang and Jian-Guo Li

Graphical Abstract

For metal oxides doped carbon aerogel (CA), the n-type and p-type semiconductors exhibited different electrocatalytic effect for phenol removal, and the former has higher effect.

695 A New Method for the Determination of Creatinine in Urine Samples Based on Disposable Pipette Extraction Aline R. Fernandes, Paulo S. de Souza, Anselmo E. de Oliveira and Andréa R. Chaves

Graphical Abstract

A simple, sensitive and reliable DPX/LC-UV (disposable pipette extraction using liquid chromatography with ultraviolet detection) method for the rapid determination of creatinine levels in urine samples.



1-(4-substituted)phenyl-1*H*-imidazole Derivatives as Open-Chain Analogues of 7-Alkoxyl-4,5-dihydro-imidazo Sl online [1,2-a]quinolines

Xian-Yu Sun, Mei-Yu Liu, Chun-Yan Zhong, Gui-Lin Zheng, Ming-Yue Lv, Bo-Tao Jing, Chun-Yuan Pan and Xin Wang

Graphical Abstract An outstanding compound was found to possess slightly more potent antibacterial activity against several bacterial strains than the reference drugs.



C₅H₁₁O

15

Leading compound

MIC against S. aureus: 8 nmol mL⁻¹ ClogP: 4.89 (ACD/Labs)



100

Bone

708

HR-MAS NMR Allied to Chemometric on Hancornia speciosa Varieties Differentiation Igor S. Flores, Andressa K. Silva, Leonnardo C. Furquim, Carlos F. S. Castro, Lazaro J. Chaves, Rosane G. Collevatti and Luciano M. Lião



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Design, Synthesis, Biological Evaluation and Molecular Modeling Studies of Novel Eugenol Esters as Leishmanicidal Agents

Chemometric analyses of ¹H high-resolution magic angle spinning nuclear magnetic resonance (¹H HR-MAS NMR) data for the chemotaxonomic investigation of *Hancornia speciosa* (mangaba) varieties.

SI online Camila M. Coelho, Thiago dos Santos, Poliany G. Freitas, Juliana B. Nunes, Marcos J. Marques, Camila G. D. Padovani, Wagner A. S. Júdice, Ihosvany Camps, Nelson J. F. da Silveira, Diogo T. Carvalho and Marcia P. Veloso

Graphical Abstract

Graphical Abstract

Synthesis of novel eugenol esters designed to inhibit the Leishmania rCPB 2.8 enzyme and *in vitro* evaluation of their biological activity. The molecular modeling study investigated the possible mechanisms of activation and inhibition exerted by some of these compounds on the enzyme rCPB 2.8.



729 Development and Validation of a Rapid and Reliable RP-HPLC-PDA Method for the Quantification of Six Diterpenes in Copaifera duckei, Copaifera reticulata and Sl online Copaifera multijuga Oleoresins

Luiza J. Carneiro, Thamires C. Bianchi, Jonas J. M. da Silva, Larissa C. Oliveira, Carly H. G. Borges, Danieli C. Lemes, Jairo K. Bastos, Rodrigo C. S. Veneziani and Sérgio R. Ambrósio

Graphical Abstract

Development and validation of a rapid and reliable reversed-phase highperformance liquid chromatography with photodiode array detection (RP-HPLC-PDA) method for quantifying six diterpenes in three species of Brazilian *Copaifera* oleoresins: *C. duckei*, *C. reticulata* and *C. multijuga*.





SI online Bruna S. Terra, Pedro H. C. da Silva, Anna Tramarin, Lucas L. Franco, Elaine F. F. da Cunha, Fernando Macedo Junior, Teodorico C. Ramalho, Manuela Bartolini, Maria L. Bolognesi and Ângelo de Fátima

Graphical Abstract Two hybrids containing the indanone-piperidine moiety of donepezil and lipoic acid scaffolds were synthesized. One hybrid displayed moderate inhibitory activity against hAChE and greater activity against hBuChE. It also showed a good antioxidant activity, exhibiting better ability in scavenging 2,2-diphenyl-1-picrylhydrazyl (DPPH) radicals than lipoic acid.







A fast and simple analytical method was firstly proposed for the determination of iron (Fe) in crude and refined vegetable oil samples by employing the conventional flame atomic absorption spectrometry (FAAS) technique and microemulsification as sample preparation procedure.



757 Magnetic Solid-Phase Extraction Combined with Dispersive Liquid-Liquid Microextraction Followed by HPLC for **Determination of Four Aromatic Amines Released from Azo Dyes in Paper Samples**

Xiaolan Li, Dongling Meng, Ruiqi Liu and Yaling Yang

Graphical Abstract

As shown in the figure, *n*-octanol, which was used as the extractant, and hydrophobic oleic acid modified Fe_3O_4 nanoparticles ($Fe_3O_4@OA NPs$), as an efficient adsorbent, were applied to retrieve the primary aromatic amines (PAAs)-containing n-octanol in the dispersive liquid-liquid microextraction (DLLME) step.



766

Antimicrobial Activity of Paepalanthus planifolius and its Major Components against Selected Human Pathogens Marcelo R. de Amorim, Felipe Hilário, Paulo T. Sano, Sl online Tais M. Bauab and Lourdes C. dos Santos



Graphical Abstract New naphthopyranone dimer named planifoliusin A isolated from Paepalanthus planifolius.



SI online

Targeted-Analysis of β-Carboline Alkaloids in Passionfruit ("Maracujá") by SBSE(PDMS)-LC/Flu and UHPLC-MS Vítor F. Freire, Gabriela R. Silva and Janete H. Yariwake



Graphical Abstract

β-Carboline alkaloids were identified in passionfruit by using UHPLC-MS (ultrahigh performance liquid chromatography-mass spectrometry) and SBSE(PDMS) (stir bar sorption extraction using polydimethylsiloxane as stationary phase) techniques.

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nanocomposites.





A Convenient and Efficient Method for the Synthesis of a Novel Series of N-Butyl-1,4-oxazino[2',3':4,5]pyrano [3,2-c]quinolinones

Sl online Hany M. Hassanin and Mohamed M. Hassan



Graphical Abstract Starting from 3-amino and/or 3-nitro-4-hydroxypyranoquinolindione, some novel 1,4-oxazinopyranoquinolinone derivatives have been synthesized.

801 Development and Validation of Liquid Chromatography-Tandem Mass Spectrometry Methods for Determination of Beta-Lactams, Macrolides, Fluoroquinolones, Sulfonamides and Tetracyclines in Surface and Drinking Water from Rio de Janeiro, Brazil

> Mychelle A. Monteiro, Bernardete F. Spisso, Rosana G. Ferreira, Mararlene U. Pereira, Jônatas V. Grutes, Bárbara R. G. de Andrade and Luiz A. d'Avila

Graphical Abstract Antibiotics in the aquatic environment are present at low level. This method was applied for quantification of 46 analytes. The validation tests showed good performance for the surface and drinking water. The method was applied to evaluate these compounds in samples from Rio de Janeiro.





SI online Nairley C. S. Firmino, Francisco S. O. Alexandre, Mayron A. de Vasconcelos, Alison J. S. Conrado, Francisco V. S. Arruda, Edilberto R. Silveira and Edson H. Teixeira

Graphical Abstract Three antibacterial 3,4-*seco*-diterpenes were isolated from hexane extracts of roots of individual specimens of *Croton blanchetianus* Baill.



823 Interlaboratory Comparison for the Characterization of a Brazilian Mussel Reference Material Edson G. Moreira, Marina B. A. Vasconcellos, Vera A. Maihara, Marília G. M. Catharino and Mitiko Saiki

> Graphical Abstract Production of a mussel reference material: from the living organism to certified mass fractions in bottles.

831 A New, Friendlier Methodology to Determine the Average Manganese Valence in Li_xMn₂O₄ Spinels Using Atomic Absorption Spectrometry and Molecular Absorption Spectrophotometry

> João P. Silva, Ricardo M. Silva, Sonia R. Biaggio, Nerilso Bocchi and Romeu C. Rocha-Filho

Graphical Abstract

Precise average manganese valences (v) for Mn oxides are attained spectroscopically. When the oxides react with Fe²⁺, Mn^{v+} is reduced to Mn²⁺; thence [Mn²⁺] is determined by AAS and excess [Fe²⁺] by MAS (after Fe²⁺ complexation with *o*-phenanthroline), enabling the determination of v.



838 Structures, Stabilities, Reactivities, and (Hyper)Polarizabilities of Small Gold Clusters Francisco E. Jorge and Alexsandro S. Santos

 $\label{eq:Graphical Abstract} Graphical Abstract DKH2-B3PW91/DZP+1d-DKH optimized ground state electronic structures for the gold clusters, Au_n (n = 3-8).$



845 Synthesis, Characterization and Catalytic Evaluation of Magnetically Recoverable SrO/CoFe₂O₄ Nanocatalyst for Biodiesel Production from Babassu Oil Transesterification Milton S. Falcão, Marco A. S. Garcia, Carla V. R. de Moura, Sabrina Nicolodi and Edmilson M. de Moura

Graphical Abstract

A very efficient SrO-based magnetic heterogeneous catalyst was developed in the studies presented herein. Biodiesel was produced from babassu oil transesterification with high yields in four catalytic cycles.





Theoretical Study of the Interaction of 1,2-Dithiolene Ligands with the Mg²⁺ and Ca²⁺ Aquacations: Electronic, Geometric 🔀 and Energetic Analysis

Sl online Glauber S. Melengate, Stanislav R. Stoyanov, Daniel G. S. Ouattrociocchi, Leonardo M. da Costa and Glaucio B. Ferreira



Graphical Abstract The interaction strength order is quantified in terms of the ΔH and ΔG of substitution of four water molecules from the $[Ca(H_2O)_6]^{2+}$ by bidentate dithiolene ligands.

Short Report

873 Comparison between Ultrasound Assisted Extraction and Microwave Digestion in the Determination of Arsenic in Edible Grains

Roberto V. Ribeiro, Júlia C. Vieira, Fabiana A. Lobo and Roberta E. S. Froes-Silva

Graphical Abstract

Comparison between microwave digestion and ultrasound assisted extraction (UAE) was made. UAE presents better performance compared to microwave digestion in arsenic extraction. Accuracy performance was close to 100% for all three methods developed. Bean samples cultivated in impacted areas presented 0.3 µg g⁻¹ of arsenic concentration.



881 Absolute Configuration of Clemateol

Marcelo Pedroso, Adriana Z. Gehn, Mateus L. Stivanin, Enrique L. Larghi, Robert A. Burrow, Jackson A. L. C. Resende, SI online Ubiratan F. da Silva, Marco A. Mostardeiro,

Ionara I. Dalcol and Ademir F. Morel

Graphical Abstract

The absolute stereochemistry of clemateol was established on the basis of detailed NMR spectroscopic evidence $({}^{3}J_{H \cdot H}$ analysis, derivatization as Mosher's esters and NOESY) and also by resonance scattering effects in the single crystal X-ray diffraction experiment of its (R)-mandelic acid ester derivative.





Dayana M. Santos, Mike Williams, Rai Kookana and Mary R. R. de Marchi



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Graphical Abstract Solid phase microextraction (SPME) fibers for use as passive sampler of endocrine disrupting chemicals as triclosan, bisphenol A and 17α -ethinylestradiol in seawater.