JBCS

ISSN 0103-5053

Journal of the Brazilian Chemical Society

Vol. 29, No. 1, January, 2018

Cover Picture



With a suitable cetyltrimethylammonium bromide (CTAB) model, we carried out molecular dynamics (MD) calculations that were able to describe most of the surfactant behavior as aggregates (micelles) in aqueous solution, as well as its interaction and molecular arrangement pattern on gold surface. Details are presented in the Article **Molecular Dynamics Simulations of Cetyltrimethylammonium Bromide (CTAB) Micelles and their Interactions with a Gold Surface in Aqueous Solution** by *José Adriano da Silva, Roberta P. Dias, Gabriel C. A. da Hora, Thereza A. Soares and Mario R. Meneghetti* on page 191.

Contents

Editorial

¹ Announcing Changes in the Editorial Board Paulo Cezar Vieira

Articles



Preparation and Performance of an Estradiol Templated Magnetic Sphere of Molecularly Imprinted Cryogel 🛃 Jian Wang, Lili Tian, Yanan Yan, Yaru Liu, Yan Zhang and

SI online Chun Yang



Graphical Abstract In this paper we describe the synthesis of estradiol templated magnetic molecularly imprinted cryogel. The excellent selective adsorption performance, solid phase extraction and chromatographic performances of the MMIC (magnetic molecularly imprinted cryogel) were investigated.





Withanolides from Leaves of Nicandra physalodes Diego A. S. Carrero, Pedro H. J. Batista, Luciana G. S. Souza, Francisco C. L. Pinto, Mayron A. de Vasconcelos, Edson H. Teixeira, Kirley M. Canuto, Gilvandete M. P. Santiago,

SI online Edilberto R. Silveira and Otília D. L. Pessoa

Graphical Abstract

Five new withanolides, in addition to six others previously reported, were isolated and characterized from the leaf acetone extract of Nicandra physalodes.



An Appraisal on the Source-to-Sink Relationship in Plants: an Application of Desorption Electrospray Ionization Mass Spectrometry Imaging

Slonline Julia R. L. Freitas, Pedro H. Vendramini, Júlio O. F. Melo, Marcos N. Eberlin and Rodinei Augusti

Graphical Abstract

Chemical images of carbohydrates and amino acids/ureides generated from Mentha × piperita leaves at distinct maturation stages and obtained upon the application of the desorption electrospray ionization mass spectrometry imaging (DESI-MSI) technique.



Nicandra physalodes





24 Aqueous Ultrasound-Assisted Extraction for the Determination of Fluoroquinolones in Mangrove Sediment by High-Performance Liquid Chromatography and Fluorescence Detector

Mônica A. Neves, Gilmar S. Silva, Natilene M. Brito, Karla C. M. Araújo, Edmar P. Marques and Lanna K. Silva

Graphical Abstract Analytical methodology for the determination of antibiotics in mangrove sediments in an estuarine system.



Kaolinite 🔀 Ding Wang, Qinfu Liu, Dandan Hou, Shuai Zhang, Sl online Peng Guo and Hongfei Cheng

Improved Method for Preparation of Methoxy-Modified

Schematic representation of the transformation from Kaol to Kaol-BTAC. The time required for preparation of methoxy-modified Kaol was shortened by more than fifty percent, and the obtained products could

be used for further process without any negative impact.





Simple and Fast Method for Identification and Quantification of Anthocyanidins in Berries by Ultra Performance Liquid Chromatography-Mass Spectrometry

SI online Julianna M. Vagula, Nayane M. Sinosaki, Marcos A. S. Ribeiro, Thiago Magon, Janksyn Bertozzi, Eduardo C. Meurer, Oscar O. Santos Junior and Jesuí V. Visentainer

Graphical Abstract

Graphical Abstract

This work aim is to identify and quantify three different anthocyanidins in six different berries and shows the elucidation of a general fragmentation mechanism.



45 Effect of Acetonitrile and N.N-Dimethylformamide on the Formation of Poly(ethylene oxide)-Sodium Alkyl Sulfate hte Aggregates

Sl online Guilherme M. D. Ferreira, Gabriel M. D. Ferreira, Maria C. Hespanhol, Álvaro J. P. Agudelo, Jaqueline P. Rezende, Ana C. S. Pires and Luis H. M. Silva

Graphical Abstract

Acetonitrile and N,N-dimethylformamide modify the water tridimensional structure in the solvation shells of sodium alkyl sulfates and poly(ethylene oxide) without altering the relative stability of the surfactant aggregates formed in the absence and in the presence of the polymer.



Cosolvent changes hydration shell $\downarrow \Delta H_{agg}(int)$

58 Synergistic Effect of 4A Zeolite from Rice Husk Ash without Aging Time and Silane on the Adhesion Properties of a Warm Mix Asphalt

Paula C. Arroyo-Martínez, Norma A. Sánchez-Flores, María E. Villafuerte-Castrejón and Rodrigo Vivar-Ocampo

Graphical Abstract 4A zeolite synthesized from rice husk by microwave-assisted hydrothermal synthesis without aging time increases the effect of the antistripping additive.





Graphical Abstract Catalytic activity profiles of 10FexMn/AC (x = 1, 3, 5) catalysts with different Fe and Mn molar ratios.





Heteropoly Tungstate Supported on Metal Oxide Catalysts for Liquid Phase Oxidation of Benzyl Alcohol with Hydrogen Peroxide

Sl online Han Xiaoxiang, Kuang Yingying, Xiong Chunhua, Tang Xiujuan, Chen Qing, Wang Kuiwu, Hung Chin-Te, Liu Li-Li and Liu Shang-Bin

> Graphical Abstract Phosphotungstic acid supported ceria shows excellent catalytic activity for oxidation of benzyl alcohol to benzaldehyde due to Brønsted-Lewis acid synergy effect.





125 Nonanoic Acid-Coated Magnetite Nanoparticles for Separation and Preconcentration of Lead and Copper in Tobacco Samples prior to Flame Atomic Absorption **Spectrometry Determination**

Shouai Feng, Hong Liu, Jiangfeng Huang, Jingjing Wu, Kang Wei, Xiaolan Li, Dongling Meng, Jiao Zhao and Yaling Yang

Graphical Abstract

evaluated against human cancer cells.

Nonanoic acid-coated magnetic Fe₃O₄ nanoparticles were used as adsorbents for preconcentration and separation of Cu and Pb. Methanolnitric acid was used as eluent for desorption of Cu and Pb, finally detected by flame atomic absorption spectrometry.



analogue



Synthesis of New trans-Dehydrocrotonin Nitrogenated Derivatives and their Cytotoxic and DNA-Topoisomerase I Inhibitory Activities

SI online Andressa Esteves-Souza, Kenia Pissinate, Maria A. M. Maciel and Aurea Echevarria



Graphical Abstract Synthesis of new trans-dehydrocrotonin nitrogenated derivatives, and in vitro evaluation of cytotoxic, and DNA-topoisomerase I activities.



New Organomineral Complex from Humic Substances Extracted from Poultry Wastes: Synthesis, Characterization and Controlled Release Study

SI online Amanda M. P. Santos, Alexandre C. Bertoli, Ana Carolina C. P. Borges, Raphael A. B. Gomes, Jerusa S. Garcia and Marcello G. Trevisan



Graphical Abstract

The humic and fulvic acids extracted from poultry manure are complexed in Cu²⁺, Zn²⁺ and Fe²⁺ and taken to a release test in contact with buffer solution.



Graphical Abstract

Invasive aquatic plants like water hyacinth is one of the major rapid growth plant in the planet and represent a water environmental problem. Through micropyrolysis experiments we can evaluate the potential to use this biomass to produce biofuels or fine chemicals.



159 Synthesis of New Conjugates 1*H*-Pyrazolo[3,4-*b*]pyridinephosphoramidate and Evaluation against *Leishmania amazonensis*

Graphical Abstract

1H-Pyrazolo[3,4-b] pyridine phosphoramidates were synthesized and evaluated against *Leishmania amazonensis* promastigotes *in vitro*.





168 Irrigation and Light Access Effects on *Coffea arabica* L. Leaves by FTIR-Chemometric Analysis Patrícia M. Sanchez, Elis D. Pauli, Guilherme L. Scheel,

Patricia M. Sanchez, Elis D. Pauli, Guilherme L. Scheel, Miroslava Rakocevic, Roy E. Bruns and Ieda S. Scarminio

Coffea arabica L. leaf extracts, grown under different environmental conditions, were analyzed by FTIR with chemometric tools. It was possible to discriminate leaves from different microclimates by bands related to carbohydrates, amino acids, lipids and caffeine.

SI online Antonia C. R. F. Medeiros, Julio C. Borges, Klaus M. Becker, Raquel F. Rodrigues, Leonor L. Leon, Marilene Canto-Cavalheiro, Alice M. R. Bernardino, Marcos C. de Souza and Leandro F. Pedrosa



185

Synthesis and in vitro Antiproliferative Activity of Flavone and 6-Hydroxyflavone Oxime Ethers Derivatives 🔀 John E. Díaz, Diana C. Martinez, Lina V. López,

Sl online Gina M. Mendez, Ricardo Vera and Alix E. Loaiza



H 1b. R = OH; 3a. R = H, R₁ = H 3b. R = H, R₁ = C₀H₅ 3c. R = H, R₁ = α-B/C₀H₄ 3d. R = H, R₁ = B/C=CH₂ 3a. R = H, R₁ = HC=C(CH₃)₂ 3d. R = H, R₁ = HC=CHC₆H₅ 3g. R = OH, R₁ = H 3b. R = OH, R₁ = C₀H₅ 3d. R = OH, R₁ = B/C=CH₂ 3k. R = OH, R₁ = HC=C(CH₃)₂ 3l. R = OH, R₁ = HC=CHC₀H₅

Graphical Abstract The synthesis of a series of O-alkyl oximes of flavone and 6-hydroxyflavone using a simple experimental protocol is reported. Cytotoxicity of all compounds was evaluated against MDA-MB-231, PC-3, A-549 and MRC-5 cells. The best IC₅₀ value was obtained for 6-hydroxyflavone (3.4 µM) against MDA-MB-231.

Analytical Strategies for Determination and Environmental Impact Assessment of Inorganic Antimony Species in Natural





Graphical Abstract

The inorganic antimony speciation in natural waters was evaluated by hydride generation atomic fluorescence spectrometry (HG AFS).

191

Molecular Dynamics Simulations of Cetvltrimethylammonium Bromide (CTAB) Micelles and their Interactions with a Gold Surface in Aqueous Solution Sl online José Adriano da Silva, Roberta P. Dias, Gabriel C. A. da Hora,

Thereza A. Soares and Mario R. Meneghetti

Graphical Abstract MD simulations of: CTAB micelles in water (left) and CTAB micelles adsorbed on a gold surface in aqueous solution (right).



Short Reports





Graphical Abstract The image shows the system used to continuously monitor the transesterification reaction.

205	New Method for Carotenoid Extraction and Analysis by
	HPLC-DAD-MS/MS in Freeze-Dried Citrus and Mango Pulps
	Fabiane C. Petry and Adriana Z. Mercadante

Carotenoid Rich in epoxycarotenoids and organic acids X analysis in citrus is still a Epoxy-furanoid rearrangement: Artifacts challenge! A NEW METHOD WAS DEVELOPED AND VALIDATED Liquid-liquid partition Ethyl acetate and methanol as solvents 9 💥 centrifugation Addition of a mild neutralizing agent Carotenoids from freeze-dried orange and mango pulps were analyzed by HPLC-DAD-MS/MS

Graphical Abstract

A new fast methodology for extraction and quantitative analysis of carotenoids from freeze-dried orange and mango pulps was developed and validated. A detailed identification and quantification, by HPLC-DAD-MS/MS, of carotenoids detected in such matrices are also given.