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# Journal of the Brazilian Chemical Society Vol. 26, No. 11, November, 2015

**Cover Picture** 



The number of antibiotic-resistant microbes increases each year, whereas the number of new antibiotics does not follow the same rate, encouraging different surveys focusing on new active substances. From an expedition into the Amazon Rain Forest different green-tree frog (*Hypsiboas cinerascens*) specimens were captured and chemically studied aiming the discovery of new antimicrobial substances. Details are presented in the Article **Cinerascetins, New Peptides from** *Hypsiboas cinerascens***: <b>MALDI LIFT-TOF-MS/MS** *de novo* **Sequence and Imaging Analysis** by *Richardson A. Almeida, Marcelo Gordo, Felipe M. A. da Silva, Rafael C. de Araújo, Marcelo H. S. Ramada, Fernando Y. Abrão, Túlio O. G. Costa, Hector H. F. Koolen, Afonso D. L. de Souza and Carlos Bloch Jr.* on page 2290.

# Contents

## Editorial

2169 Chemistry of Our Oceans Vanessa Hatje

## Communication

2171

Metal Oxide/Gold Hybrid Nanocomposites as Electrocatalysts for Alkaline Air Electrodes Anielli M. Pasqualeti, Francisca E. R. Oliveira and SI online Fabio H. B. Lima

**Graphical Abstract**  $MnCo_2O_4/Au$  exhibited a synergistic effect boosting the oxygen reduction and evolution. In situ X-ray absorption near edge structure (XANES) revealed that  $Mn^{\mbox{\tiny III}}\mbox{-}Co^{\mbox{\tiny II}}$  play a role in the reduction. Au induced the increase in the Co<sup>IV</sup> amount, favoring the oxygen evolution

## **Review**

2175 Zinc, Lithium and Magnesium Carbenoids: Chemical Properties and Relevant Applications in Organic Synthesis Rodolfo H. V. Nishimura, Valter E. Murie, Rafael A. Soldi, João L. C. Lopes and Giuliano C. Clososki

**Graphical Abstract** The ambiphilic character of carbenoids, represented by the chinese yin yang, shows how apparently opposite forces can be complementary in organic synthesis

## Articles

2189 Volatile Organic Compounds from Filamentous Fungi: a Chemotaxonomic Tool of the Botryosphaeriaceae Family Francisco C. Oliveira, Francisco G. Barbosa, Jair Mafezoli, Maria C. F. Oliveira, André L. M. Camelo, Elisane Longhinotti,

SI online Ari C. A. Lima, Marcos P. S. Câmara, Francisco J. T. Gonçalves and Francisco C. O. Freire

## **Graphical Abstract**

Volatile organic compounds from ten endophytic fungal species belonging to the Botryosphaeriaceae family were extracted by headspace-solid phase micro-extraction (HS-SPME) and analyzed by gas chromatography-mass spectrometry (GC-MS)

2195 Binary Micellar Solutions of Poly(Ethylene Oxide)-Poly(Styrene Oxide) Copolymers with Pluronic<sup>®</sup> P123: Drug Solubilisation and Cytotoxicity Studies

Samira A. Oliveira, Carolina L. Moura, Igor M. Cavalcante, Amanda Araújo Lopes, Luzia K. A. M. Leal, Nilce V. Gramosa, Maria E. N. P. Ribeiro, Francisco C. F. França, Stephen G. Yeates and Nágila M. P. S. Ricardo

## **Graphical Abstract**

P123 and EmSn binary micelles presented thermorreversible gelation, low critical micelle concentration (cmc), good drug solubilisation capacity and no citotoxicity

2205 Determination of Parabens in Surface Water from Mogi Guaçu River (São Paulo, Brazil) Using Dispersive Liquid-Liquid Microextraction Based on Low Density Solvent and LC-DAD SI online

Carlos A. Galinaro, Fabiana M. Pereira and Eny M. Vieira

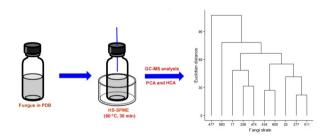
### **Graphical Abstract**

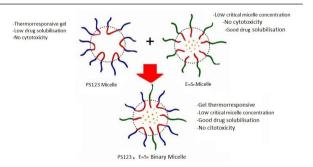
This study has demonstrated the successful analysis of parabens on surface water samples, collected from Mogi Guaçu River (São Paulo state, Brazil), by dispersive liquid-liquid microextraction (DLLME) based on low density solvent (LDS) combined with liquid chromatography with diode array detection (LC-DAD)

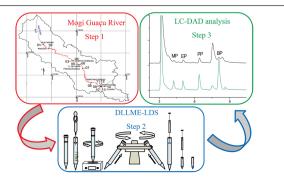
-0.8 -0.6 -0.4 -0.2 0.0 0.2 E / V vs. Hg/HgO/OH

-1.0





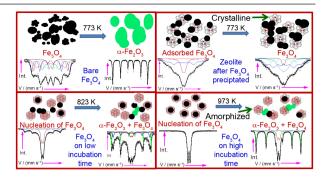




## Vol. 26, No. 11, 2015

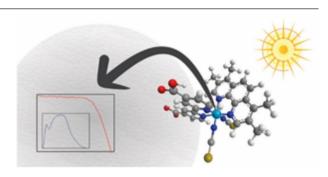
2214 Facile Method to Tune the Particle Size and Thermal Stability of Magnetite Nanoparticles Loushambam H. Singh, Sudhanshu S. Pati, Maria J. A. Sales, Edi M. Guimarães, Aderbal C. Oliveira and

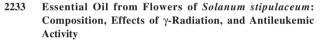
Vijayendra K. Garg



**Graphical Abstract** Zeolite confines the growth of the magnetite nanoparticles and provides stability, which prevents from agglomeration and oxidation leading to structural transformation

2224 Effects of Methyl-Substituted Phenanthrolines on the Performance of Ruthenium(II) Dye-Sensitizers Andressa V. Müller, Poliana S. Mendonça, Stéphane Parant, Thibaut Duchanois, Philippe C. Gros, Marc Beley and André S. Polo





Aura M. B. Osorio, Thiago M. Silva, Lucienir P. Duarte, Vany P. Ferraz, Márcio T. Pereira, Maria O. Mercadante-Simões, Fernanda C. G. Evangelista, Adriano P. Sabino and Antônio F. C. Alcântara

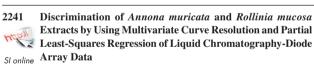
Cis-[Ru(Me<sub>4</sub>-phen)(dcbH<sub>2</sub>)(NCS)<sub>2</sub>] was prepared, characterized and employed in dye-sensitized solar cells. The presence of four methyl groups on 1,10-phenanthroline modulates its ground and excited states

and the ability to convert sunlight into electrical energy

#### Graphical Abstract

Graphical Abstract

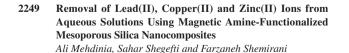
The essential oil composition of y-irradiated flowers of Solanum stipulaceum was analyzed by gas chromatography (GC). The cytotoxicity of essential oils from non-irradiated and irradiated flowers was also studied



Sabrina Afonso, Pablo L. Pisano, Fabiano B. Silva, Ieda S. Scaminio and Alejandro C. Olivieri

#### **Graphical Abstract**

Discrimination of Annona muricata and Rollinia mucosa samples processed by multivariate curve resolution-alternating least-squares (MCR-ALS) and discriminant-unfolded partial least-squares (D-UPLS) of high-performance liquid chromatography with diode array detection (HPLC-DAD) data

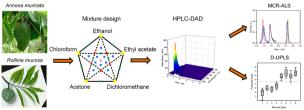


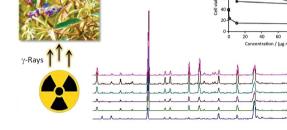
NH: NH<sub>2</sub> NH, MCM-4 APTES NH NH. MCM-41 coated Fe<sub>3</sub>O<sub>4</sub> NH: NH. NH. ICP

Si-NH2···Pb(II)

Graphical Abstract Fe<sub>3</sub>O<sub>4</sub> nanoparticles were coated with mesoporous silica, MCM-41, and then amino-functionalization was performed on the MCM-41 surface by 3-aminopropyltriethoxysilane through the silanization reaction with hydroxyl groups of MCM-41. Fe<sub>3</sub>O<sub>4</sub>@MCM-41-NH<sub>2</sub> was used for extraction of some toxic metal ions from aqueous solutions











## Catalytic Activity of a Titanium(IV)/Iron(II) Heterometallic Alkoxide in the Ring-Opening Polymerization of ε-Caprolactone and rac-Lactide

Sl online Siddhartha O. K. Giese, Cristiano Egevardt, André Luis Rüdiger, Eduardo L. Sá, Thiago Alessandre Silva, Sônia F. Zawadzki, Jaísa F. Soares and Giovana G. Nunes

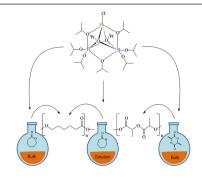
#### Graphical Abstract

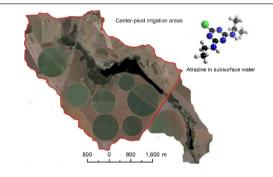
Graphical Abstract

subsurface water

The heterometallic complex [FeCl{Ti,(O'Pr),}] was employed as initiator of ring-opening polymerization of  $\varepsilon$ -caprolactone and *rac*-lactide in bulk and in solution. The catalytic performance of the heterometallic complex was compared to the activities of other titanium(IV) and iron(II) complexes

2269 Monitoring of Pesticide Residues in Surface and Subsurface Waters, Sediments, and Fish in Center-Pivot Irrigation Areas Aderbal A. Rocha, Sérgio H. Monteiro, Graziela C. R. M. Andrade, Franz Z. Vilca and Valdemar L. Tornisielo





# 2279

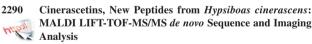
## Synthesis and Insecticidal Activity of Lactones Derived from Furan-2(5H)-one

This work is about a study of pesticide residue contamination in surface and subsurface waters, sediments and fish of center-pivot irrigation areas. Atrazine was observed below the method quantitation limit in

🔀 Milena G. Teixeira, Elson S. Alvarenga, Mirian F. Pimentel and SI online Marcelo C. Picanço

#### Graphical Abstract

Besides the efficiency against insect pests, novel agrochemicals should preferably provide selectivity to non-target species. Therefore, the lactones synthetized in this work are promising as potential novel agrochemicals for the integrated pest management



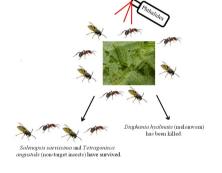
Sl online Richardson A. Almeida, Marcelo Gordo, Felipe M. A. da Silva, Rafael C. de Araújo, Marcelo H. S. Ramada, Fernando Y. Abrão, Túlio O. G. Costa, Hector H. F. Koolen, Afonso D. L. de Souza and Carlos Bloch Jr.

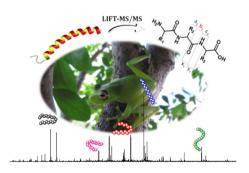
#### **Graphical Abstract**

In this work, new peptides named cinerascetins were identified from skin secretion of the Hypsiboas cinerascens. Imaging analysis localized the peptides on the dorsal tissue. Synthetic cinerascetin-01 was tested against some bacteria and fungi presenting satisfactory antimicrobial activities



Synthesis of 3-(1H-1,2,3-Triazol-1-yl)-2-(arylselanyl) pyridines by Copper-Catalyzed 1,3-Dipolar Cycloaddition of 2-(Arylselanyl)-3-azido-pyridines with Terminal Alkynes Sl online Ricardo F. Schumacher, Patrick B. Von Laer, Eduardo S. Betin, Roberta Cargnelutti, Gelson Perin and Diego Alves

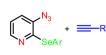




Cu(OAc)<sub>2</sub>.H<sub>2</sub>O (5%)

Sodium ascorbate (10%)

THF/H2O (1:1), r.t., air



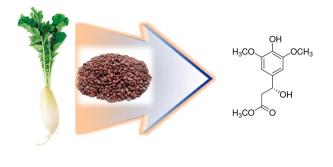


Graphical Abstract The synthesis of 3-(1H-1,2,3-triazol-1-yl)-2-(arylselanyl)pyridines by copper-catalyzed cycloaddition reaction is presented here



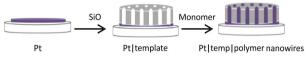
Chemical Constituents of the Seeds of Raphanus sativus and their Biological Activity Ki Hyun Kim, Eunjung Moon, Seoung Rak Lee, Kyoung Jin

SI online Park, Sun Yeou Kim, Sang Un Choi and Kang Ro Lee



**Graphical Abstract** Fifteen constituents, including a new phenolic compound, were isolated from the seeds of Raphanus sativus. Some of the isolated compounds showed moderate antiproliferative activities and significant anti-neuroinflammatory effects

2313 **Electrosynthesis and Characterisation of Polymer Nanowires** from Thiophene and its Oligomers María Angelica del Valle, Andrea C. Ramos, Fernando R. Diaz and Manuel A. Gacitua



Graphical Abstract

Graphical Abstract

and gas chromatography-mass spectrometry

Polythiophene was electrosynthesised as nanowires from the monomer and some of its oligomers on a Pt electrode previously modified with a template

A new and five known piperamides were unequivocally characterized in mixture from few amounts of semi-purified fractions from fruits, leaves, stems and roots of Piper ottonoides by using nuclear magnetic resonance

Evaluation of Monolithic and Core-Shell Columns for

Separation of Triazine Herbicides by Reversed Phase High

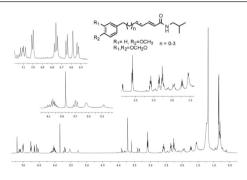
🔀 Performance Liquid Chromatography SI online Ricardo P. Urio and Jorge C. Masini

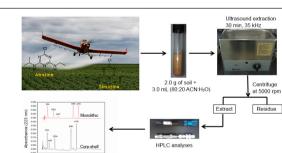


2331

## Piperamides from Piper ottonoides by NMR and GC-MS Based Mixture Analysis

Thiago Wolff, Priscila F. P. Santos, Ligia M. M. Valente, Sl online Alvicler Magalhães, Luzineide W. Tinoco, Rita C. A. Pereira and Elsie F. Guimarães

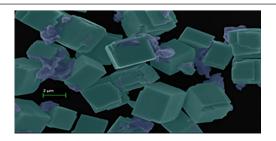




Graphical Abstract Monolithic and core-shell chromatographic columns were evaluated for separation of triazines and some of their metabolites in ultrasound extracted soil

2339 Facile Microwave-Assisted Synthesis of Lanthanide Doped CaTiO<sub>3</sub>Nanocrystals

Sandra C. Pereira, Alberthmeiry T. Figueiredo, Cristiano M. Barrado, Marcelo H. Stoppa, Yashashchandra Dwivedi, Maximo S. Li and Elson Longo



**Graphical Abstract** 

Fast synthesis of lanthanide doped CaTiO<sub>3</sub> produces a microcube-like structure and a region without well-defined morphology. The structural disorder and observed photoluminescence emission are correlated



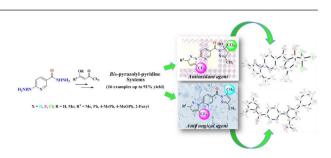
2369

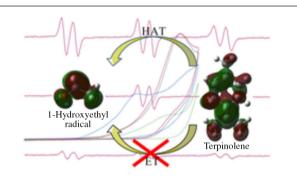
#### Synthesis, Structure Elucidation, Antioxidant and Antimicrobial Activity of Novel 2-(5-Trifluoromethyl-1Hhttp pyrazol-1-yl)-5-(5-trihalomethyl-1H-pyrazol-1-yl-1-carbonyl) SI online pyridines

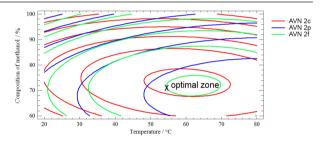
Helio G. Bonacorso, Susiane Cavinatto, Maiara C. Moraes, Everton P. Pittaluga, Luis R. Peroza, Tarcieli Venturini, Sydney H. Alves, Sílvio T. Stefanello, Félix A. A. Soares, Marcos A. P. Martins, Nilo Zanatta and Clarissa P. Frizzo

Graphical Abstract Synthesis, structure, antioxidant and antimicrobial activity evaluation of novel 2-(5-trifluoromethyl-1H-pyrazol-1-yl)-5-(5-trihalomethyl-1Hpyrazol-1-yl-1-carbonyl)pyridines bearing two distinct trihalomethyl substituted pyrazole rings

2362 Mechanism of Hop-Derived Terpenes Oxidation in Beer Natália E. C. de Almeida, Inara de Aguiar and Daniel R. Cardoso







**Graphical Abstract** 

**Graphical Abstract** 

than by an electron transfer mechanism

The optimization method which combined desirability function with response surface methodology (RSM) models was chosen to find the best extraction conditions for obtaining maximum yield of major avenanthramides from oat grain

The oxidation of hop-derived terpenes in beer has been shown to occur through a hydrogen atom abstraction by 1-hydroxyethyl radical rather

**Optimization of Parameters for Extraction of Avenanthramides** 

from Oat (Avena sativa L.) Grain Using Response Surface

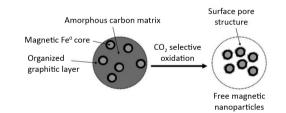
Maria Maliarova, Viera Mrazova, Michaela Havrlentova and

# Short Report

Methodology (RSM)

Jozef Sokol

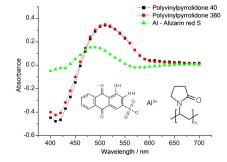
2379 Selective Oxidation of Amorphous Carbon by CO<sub>2</sub> to Produce Fe@C Nanoparticles from Bulky Fe/C Matrices Fernanda G. Mendonça, José D. Ardisson, Rochel M. Lago and Sl online Juliana C. Tristão



**Graphical Abstract**  $Fe^{0}$  cores encapsulated in a carbon matrix treated with  $CO_{2}$  to selectively oxidize the amorphous carbon and release carbon coated magnetic nanoparticles

#### 2384 Spectrophotometric Determination of Aluminium in Hemodialysis Water

Eder J. Santos, Eduardo B. Fantin, Ronei E. Paixão, Amanda B. Herrmann and Ralph E. Sturgeon



## Graphical Abstract

This work describes a simple and fast spectrophotometric method for the determination of aluminium in hemodialysis water employing alizarin red S in the presence of polyvinylpyrrolidone 40