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# **Cover Picture**



Antimicrobial resistance is a global concern because is present in every country. Bacterial biofilm is associated with many persistent infections and increased resistance to antibiotics. Diguanylate cyclase enzymes (DGC) are an attractive target for antibiofilm drug intervention. Drug repurposing strategy resulted in DGC inhibitors discovery from therapeutics drugs using the integration of computational and biochemical assays. Details are presented in the Article **Identification of Anti-Inflammatory and Anti-Hypertensive Drugs as Inhibitors of Bacterial Diguanylate Cyclases** by *Helton J. Wiggers, Édson Crusca, Éverton E. D. Silva, Juliana Cheleski, Naiara U. Torres and Marcos V. A. S. Navarro* on page 297.

# Contents

# Articles

217 Synthesis and Application of Bimetallic Zinc(II) Phenoxy-Imine Complexes as Initiators for Production of Lactide Polymers Alana L. C. Oliveira, Leonardo C. Ferreira, Marcos L. Dias,

Rodrigo S. Bitzer, Marco A. C. Nascimento, Maria de Fátima V. Marques and Laura Crociani



Graphical Abstract Bimetallic Zn<sup>II</sup> complexes with phenoxy-imine ligands were synthesized and used as initiators for lactide polymerization. L-lactide

Poly(L-lactic acid)

15

20

0.0 0.1

10 Time/h



Nanoporous Gold Surface: An Efficient Platform for Hydrogen Evolution Reaction at Very Low Overpotential Anandhakumar Sukeri and Mauro Bertotti

SI online

248

# **Graphical Abstract**

0

20- يې E -0.070

-60

-0.2 -0.1

LAuCl

Mm/ 40

A nanostructured porous gold based electrocatalyst was fabricated via a facile electrochemical approach and an excellent activity with good stability for hydrogen evolution reaction was noticed.



#### Graphical Abstract

Based on thymine-Hg^2+-thymine binding mode (T-Hg^2+-T), a sensitive aptamer biosensor was constructed by utilizing functionalized Au@Ag core-shell nanoparticles as labels for detection of Hg2+.

240 Binary Blends of Biodiesel from Macauba (Acromia aculeata) Kernel Oil with Other Biodiesels Willian L. G. da Silva, Acacia A. Salomão, Patricia T. de Souza, Marina Ansolin and Matthieu Tubino

### **Graphical Abstract**

The oil from the kernel of macauba presents high stability to oxidation, property that is transferred to its biodiesel, which also presents low cold filter plugging point. Such properties are inherited by its blends with biodiesels obtained from other vegetable oils.





Cheeses made with saffron are expected to provide an added value for consumers, due to saffron bioactive compounds. This UHPLC method seems to be useful to detect saffron crocins in dairy products.





0

-20

-60

80

-100

ò

5

cm-2 -40

Am M

Bare Au

Bare Pt NPGF

> 0.2 0.3

0.0 0.1 E/V vs RHE

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of a Heterocyclic Chalcone Jean M. F. Custodio, Cauã A. Moreira, Clodoaldo Valverde, Gilberto L. B. de Aquino, Basílio Baseia and Hamilton B. Napolitano **Graphical Abstract** The nature of crystal packing of an heterocyclic chalcone, investigated by Hirshfeld surfaces, and its potential nonlinear optical properties.



# Synthesis of 3,5-Diarylisoxazole Derivatives and Evaluation of in vitro Trypanocidal Activity

Hirshfeld Surfaces and Nonlinear Optics on Two Conformers

Aline A. N. de Souza, Viviane F. Xavier, Gleicekelly S. Coelho, SI online Policarpo A. Sales Junior, Alvaro J. Romanha, Silvane M. F. Murta, Claudia M. Carneiro and Jason G. Taylor



A series of novel substituted isoxazoles were prepared and tested for in vitro anti T. cruzi activity. The lead compound is equally as potent as reference drug benzonidazole.



278 Use of Amphiphilic Composites based on Clay/Carbon Nanofibers as Fillers in UHMWPE

# Claudilene R. Silva, Rochel M. Lago, Helena S. Veloso and

Sl online Patrícia S. O. Patricio

# **Graphical Abstract**

The more efficient interaction of the fillers based on hydrophobic surface nanostructures with the hydrophobic UHMWPE chains leading to a much higher dispersion of the filler particles throughout the polymeric matrix.





# Evaluation of the Concentration of Cu, Zn, Pb and Cr in Different Fish Species from the São Gonçalo Channel in Pelotas-RS, Brazil

Sl online Marcelo M. Alves, Aline L. Medina, Ane Martiele T. Pinto, Ana Clara N. Antunes, Pedro José Sanches Filho, Anderson S. Ribeiro and Mariana A. Vieira



**Graphical Abstract** The concentration of Cu, Zn, Cr and Pb in different species of fish collected in the estuarine and limnic regions of the São Gonçalo channel in Pelotas City were determined.





310 Surface Imprinting of Silica Gel by Methyldopa and Its Application in the Solid Phase Extraction Procedure Mohammad Taghi Vardini and Leila Mardani

# Graphical Abstract

Surface of the activated silica gel was grafted with the complex of MTD-APS. The custom made holes to the MTD remain on the surface of molecularly imprinted adsorbent.

320 Functionalization of Bentonite and Vermiculite after the Creation of Structural Defects through an Acid Leaching Process

Dorsan S. Moraes, Lucas C. R. Miranda, Rômulo S. Angélica, Geraldo N. Rocha Filho and José R. Zamian

#### Graphical Abstract

Schematic model of a 2:1 layer structure of the organofunctionalized materials present in this work, suggesting the superficial acid sites created.







**Graphical Abstract** Polymerization reaction with a nickel-based catalyst supported on SBA-15 mesoporous materials.

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334 Preparation of Tetraethylenepentamine Modified Magnetic Graphene Oxide for Adsorption of Dyes from Aqueous Solution

Xiaosheng Tang, Ping Tang and Liangliang Liu



# **Graphical Abstract**

Tetraethylenepentamine modified magnetic graphene oxide nanomaterial was prepared and it had a good adsorption ability to remove dyes in wastewater.



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Assunção

Synthesis, Antioxidant Activity, Acetylcholinesterase Inhibition and Quantum Studies of Thiosemicarbazones Larissa Sens, Aldo S. de Oliveira, Alessandra Mascarello, Inês

Sl online M. C. Brighente, Rosendo A. Yunes and Ricardo J. Nunes



**Graphical Abstract** The current study investigated the antioxidant activity, acetylcholinesterase inhibition and quantum studies of thiosemicarbazones.

353	Alkaline Solubilization of Chicken Tissues Monitored by
http://	Raman Spectroscopy Followed by Pb Determination by
11023	GFAAS

SI online Náira S. Campos, Marcone A. L. de Oliveira, Celly M. S. Izumi and Rafael A. de Sousa

#### **Graphical Abstract**

Lead content was evaluated in chicken viscera by GF AAS after solubilization with tetramethylammonium hydroxide (TMAH). Sample preparation was monitored by Raman spectroscopy and SEM-EDS.





Mass spectrometry analysis as additional tool for description and differentiation of tumor physiopathology: a comparative proteomic study between pheomorphic sarcoma, metastasis and healthy tissues.



371 Effect of Selenite and Selenate Application on Mineral **Composition of Lettuce Plants Cultivated Under Hydroponic** Conditions: Nutritional Balance Overview Using a Multifaceted Study

Emanueli do Nascimento da Silva, Mirla Cidade, Gabriel Heerdt, Rafael L. Ribessi, Nelson H. Morgon and Solange Cadore

#### Graphical Abstract

Selenate and selenite enrichment in the Veneza Roxa lettuce was carried out and the mineral composition was evaluated using ICP OES, PCA and molecular modeling. Selenate-biofortified lettuce showed a synergetic effect with S and Mo while selenite-biofortified lettuce showed a synergetic effect with Mn, P, Mg and Ca.



EE2

Degradation

products

GC-MS/MS MSTFA/TMSI



#### **Graphical Abstract**

Photocatalytic degradation of estrogens by suspended and immobilized TiO<sub>2</sub> were compared in aqueous and wastewater samples. The EE2 degradation products were monitored by GC-MS/MS.

390 Comparative Study of the Lipid Profiles of Oils from Kernels of Peanut, Babassu, Coconut, Castor and Grape by GC-FID and Raman Spectroscopy William S. Martini, Brenda L. S. Porto, Marcone A. L. de Oliveira and Antonio C. Sant'Ana

**Graphical Abstract** 

A fast evaluation of the degree of unsaturation and the presence of oxidized products in oil samples by Raman spectroscopy, through the identification of marker bands, assigned by supporting of GC-FID analyses of standard fatty acids.





Absolute Configuration of Solenopsis Piperidines is a Tool to Classify Fire Ants (Formicidae:Myrmicinae) Francisca D. S. Araújo, Marcela A. Botelho, José R. Trigo and

Sl online Anita J. Marsaioli



Graphical Abstract Chiral GC chromatogram of the peak discrimination of 2-methyl-6-undecylpiperidine trifluoroacetamide stereoisomers (synthetic standard mixture).

380



Thermal properties and kinetics of  $Al/\alpha$ -MnO<sub>2</sub> nanostructure thermite was reported in this work. According to DSC curves, the heat release and onset temperature were measured. Then the changes of activation energy on extent of conversion ( $\alpha$ ) for kinetics of  $Al/\alpha$ -MnO<sub>2</sub> thermite were obtained by using isoconversional method.





Catalytic Behaviors of  $Co^{II}$  and  $Mn^{II}$  Compounds Bearing *a*-Diimine Ligands for Oxidative Polymerization or Drying Oils

SI online Gilvan E. S. Lima, Everton V. Nunes, Roberta C. Dantas, Carlos A. de Simone, Mario R. Meneghetti and Simoni M. P. Meneghetti

> **Graphical Abstract** Metal carboxylate complex modified with nitrogen ligands used as catalyst to oxidative polymerization of drying oils.



419 Enantiomeric Ratio Changes of Terpenes in Essential Oils from Hybrid *Eucalyptus grandis* × *E. tereticornis* and its Pure Species

Cecilia Naspi, Agustín A. Costa, Alejandro Lucia, Paola G. Audino and Hector M. Masuh

# **Graphical Abstract**

Fractionation of essential oils from *Eucalyptus grandis* × *E. tereticornis*, and its parental taxa, by HPLC followed by GC-MS analysis using two columns in series, allowed to determinate the enantiomeric excesses of selected monoterpenes. Significant differences were found in the enantiomeric ratios in monoterpene alcohols between the three essential oils.



# **Short Report**

430 Fast Screening of Solvents for Simultaneous Extraction of Furfural, 5-Hydroxymethylfurfural and Levulinic Acid from Aqueous Solution Using SMD Solvation Free Energies Sl online Ellen V. Dalessandro and Josefredo R. Pliego Jr.



Graphical Abstract Automated computational screening of 178 solvents for extraction of organic chemicals from aqueous phase.