

Cover Picture

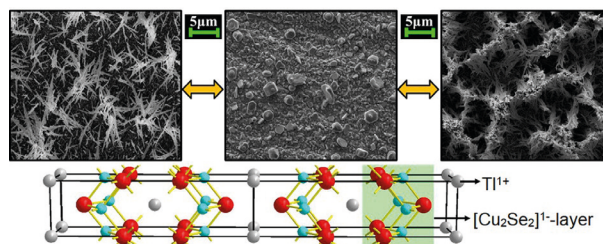


Cosmetic based on vegetable oils, such as sesame, peanut, sunflower and almonds, has beneficial properties to the human skin, and, for this reason, they are increasingly being used as moisturizers, emollients, regenerators and antioxidants, in bath oils, shampoos and hair conditioners, creams and lotions products. Nevertheless, these vegetable oils are made of high cost raw materials, and consequently they are targets of adulterations, especially with addition of soybean oil. Hence, people daily use in their body soybean oil, believing that they are taking care of their body health with other oils. This study evaluated the authenticity of Brazilian cosmetics based on vegetable oils with gas chromatography with flame ionization detection (GC-FID), and direct infusion by electrospray ionization mass spectrometry (ESI-MS). Details are presented in the Article **Assessment of Adulteration of Cosmetics Based on Vegetable Oils by GC-FID and Lipid Profile Using Direct Infusion Electrospray Ionization Mass Spectrometry (ESI-MS)** by Jessica S. Pizzo, Marília B. Galuch, Patrícia D. S. Santos, Oscar O. Santos, Lorena Visentainer, Marcos N. Eberlin and Jesuí V. Visentainer on page 2457.

Contents

Articles

- 2449 **Electrochemical Deposition of the Single Phase $Ti_xCu_{3-x}Se_2$ Thin Films**
Francisco W. S. Lucas and Lucia H. Mascaro



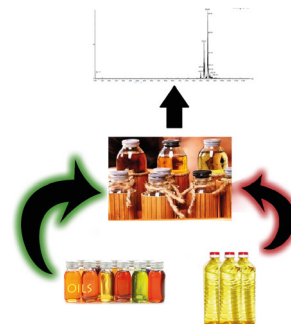
Graphical Abstract
 $TiCu_2Se_2$ texturized film was electrodeposited with [004] crystalline plane oriented parallel to the substrate surface. This texturization can also be associated with the films morphology.

2457 Assessment of Adulteration of Cosmetics Based on Vegetable Oils by GC-FID and Lipid Profile Using Direct Infusion Electrospray Ionization Mass Spectrometry (ESI-MS)

SI online Jessica S. Pizzo, Marília B. Galuch, Patrícia D. S. Santos, Oscar O. Santos, Lorena Visentainer, Marcos N. Eberlin and Jesuí V. Visentainer

Graphical Abstract

Vegetable oils have been applied to human skin for cosmetic purposes for a long time. However, they are targets of adulterations, especially with addition of oils with low cost. This study will evaluate the authenticity of Brazilian cosmetics based on vegetable oils.

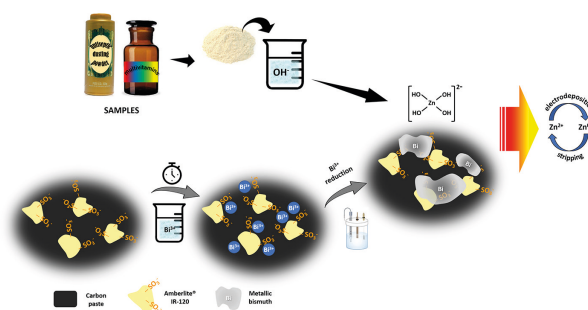


2466 Voltammetric Determination of Zn^{2+} in Antiseptic Dusting Powder and Multivitamins Using a Carbon Paste Electrode Modified with Bi Anchored on Amberlite® IR120

SI online Wilson T. Fonseca, Leandro A. R. Ribeiro, Lauro A. Pradela-Filho, Regina M. Takeuchi and André L. Santos

Graphical Abstract

Carbon paste electrodes modified with Bi anchored on Amberlite® IR120 enable fast Zn^{2+} determination in multivitamin and antiseptic dusting powder samples.

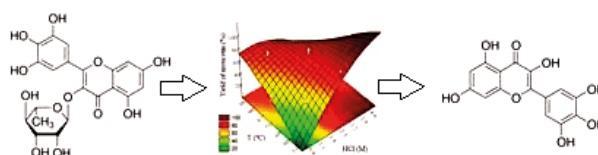


2475 Optimization of Acid Hydrolysis of Myricetin-3-O-rhamnoside Using Response Surface Methodology

Tatiana C. Tolosa, Hervé Rogez, Evaldo M. Silva and Jesus N. S. Souza

Graphical Abstract

The acid hydrolysis of glycosylated flavonols were optimized and the hydrolytic process used is effective and applicable to plant extract (*Inga edulis* leaves).

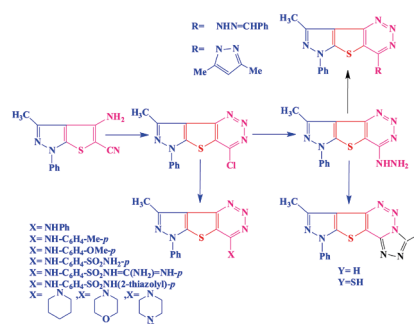


2482 A Convenient Synthesis, Reactions and Biological Activity of Some New 6H-Pyrazolo[4',3':4,5]thieno[3,2-d][1,2,3]triazine Compounds as Antibacterial, Anti-Fungal and Anti-Inflammatory Agents

SI online Remon M. Zaki, Adel M. Kamal El-Dean, Shaban M. Radwan and Ahmed F. Saber

Graphical Abstract

In the present work, we have provided an easy access for synthesis of novel thienopyrazole compounds, which were used as starting materials for building new heterocyclic systems namely: pyrazole, triazole and triazine, attached or fused to the thienopyrazole moiety that have revealed remarkable antimicrobial and anti-inflammatory activities.



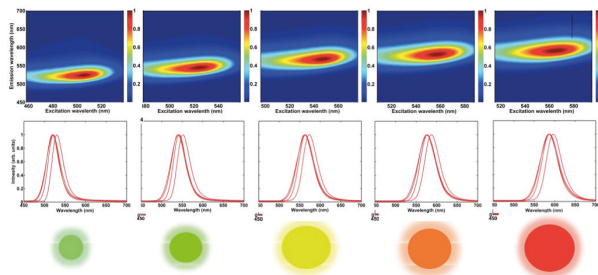
2496 Synthesis and Optical Properties of Water-Soluble CdTe:Zn²⁺ Quantum Dots Prepared by the One-Pot Approach

José C. L. Sousa, Marcelo G. Vivas, Jefferson L. Ferrari and Marco A. Schiavon

SI online

Graphical Abstract

Color map representing the emission vs. excitation wavelengths for different synthesis times of CdTe:Zn²⁺ quantum dots (QDs), and the normalized characteristic emission spectra obtained from the evolving factor analysis/multivariate curve resolution alternating least squares (EFA/MCR-ALS) method for each QD solution show the different sizes of the nanoparticles.



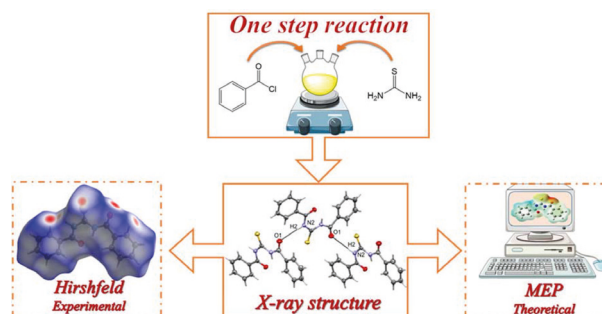
2502 Facile Synthesis and Characterization of Symmetric N-[(Phenylcarbonyl) carbamothioyl]benzamide Thiourea: Experimental and Theoretical Investigations

Rafael G. Silveira, Anderson J. L. Catão, Beatriz N. Cunha, Fernando Almeida, Rodrigo S. Correa, Luan F. Diniz, Juan C. Tenório, Javier Ellena, Aleksey E. Kuznetsov, Alzir A. Batista and Edésio Alcântara

SI online

Graphical Abstract

Simple synthesis path for obtaining a symmetric thiourea, the theoretical characterization and verification of the intermolecular interactions obtained by X-ray crystallography.

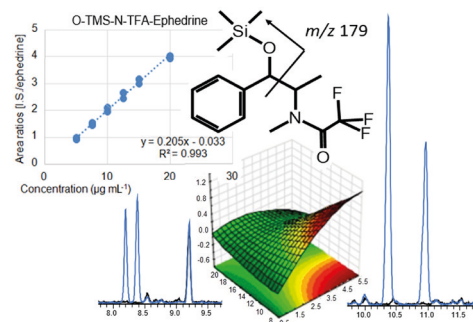


2514 Fast Ephedrine Quantification by Gas Chromatography Mass Spectrometry

Gabriel R. A. Carneiro, Andressa M. S. Silva, Raquel M. Cavalcante, Monica C. Padilha, Francisco R. de Aquino Neto, Henrique M. G. Pereira and Vinícius F. Sardela

Graphical Abstract

Straightforward method for ephedrine quantification based on gas chromatography mass spectrometry (GC-MS), without cleanup, and optimized by multivariate Doehlert matrix.



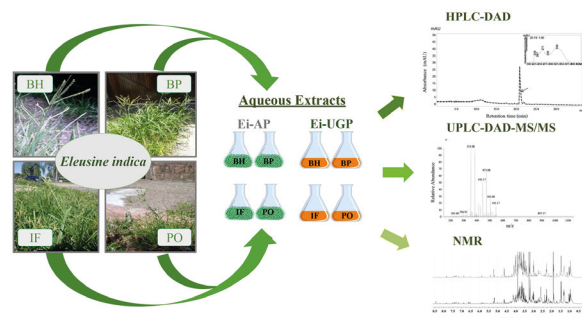
2522 Metabolite Fingerprinting and Profiling of the Medicinal Grass Eleusine indica Based on HPLC-DAD, UPLC-DAD-MS/MS and NMR Analyses

Evelyn M. C. Peñaloza, Livia M. Casanova, Ivana C. R. Leal, Paula F. de Aguiar and Sônia S. Costa

SI online

Graphical Abstract

Crude aqueous extracts of aerial and underground parts of *Eleusine indica* populations from four different localities were analyzed by high-performance liquid chromatography with diode array detection (HPLC-DAD), ultra-performance liquid chromatography with diode array detector and mass spectrometry (UPLC-DAD-MS/MS) and nuclear magnetic resonance (NMR) spectroscopy.

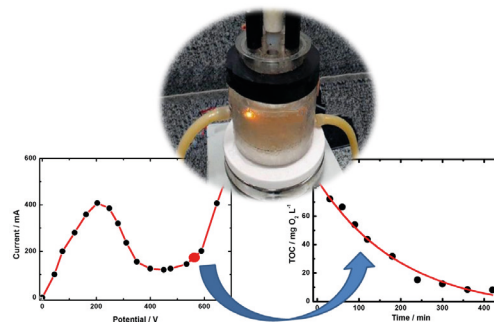


2535 Pulp Mill Effluent Treatment Using Plasma Obtained by High Voltage Electrolysis

Alexsandro A. Matias, César Reis, Efraim L. Reis,
Cláudio M. Silva, Odilaine I. C. Damasceno and
Antônio A. Neves

Graphical Abstract

The plasma is produced between two electrodes immersed in the pulp mill effluent, at 585 V and 200 mA, producing various types of reactive agents, that were used to breakdown diverse organic compounds.

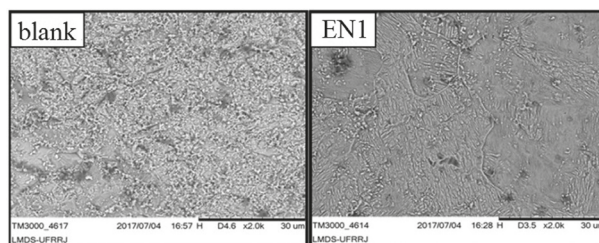


2542 β -Enaminoesters as Novel Corrosion Inhibitors for Carbon Steel in Acidic Medium

Mariana F. L. P. Carlos, Arthur Valbon, Marcelo A. Neves,
Margareth R. L. Santos and Aurea Echevarria

Graphical Abstract

American Iron and Steel Institute (AISI) 1020 carbon steel in 0.5 mol L⁻¹ HCl in absence (blank) and presence of 1×10^{-2} mol L⁻¹ ethyl-(2Z)-3-[(2-phenylethyl)amino]but-2-enoate (EN1).



2554 Virtual Screening for the Selection of New Candidates to *Trypanosoma cruzi* Farnesyl Pyrophosphate Synthase Inhibitors

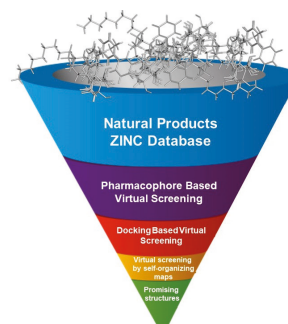


SI online

Larissa M. Oliveira, Janay S. C. Araújo, David B. Costa Júnior,
Manoelito C. dos Santos Junior, Aníbal F. Santos Júnior and
Franco H. A. Leite

Graphical Abstract

Virtual screening to select *Trypanosoma cruzi* farnesyl pyrophosphate synthase inhibitors.

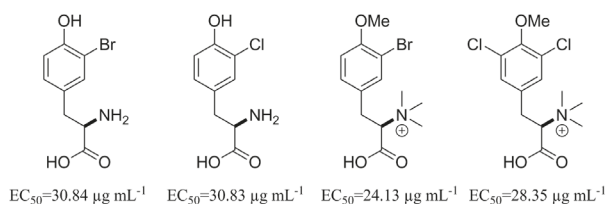


2569 Anti-Parasite and Cytotoxic Activities of Chloro and Bromo L-Tyrosine Derivatives



SI online

Manuel Pastrana Restrepo, Elkin Galeano Jaramillo,
Alejandro Martínez Martínez, Ana Mesa Arango and
Sara Robledo Restrepo



Graphical Abstract

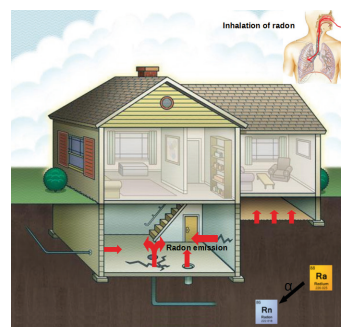
Bromo and chloro L-tyrosine derivatives actives against *L. panamensis*.

2580 Radon Levels in a Hospital in Niterói Municipality-RJ, Brazil

Camila R. Silva, Pedro P. Caldeira, Angela S. F. Nani and
Emmanuel V. Silva-Filho

Graphical Abstract

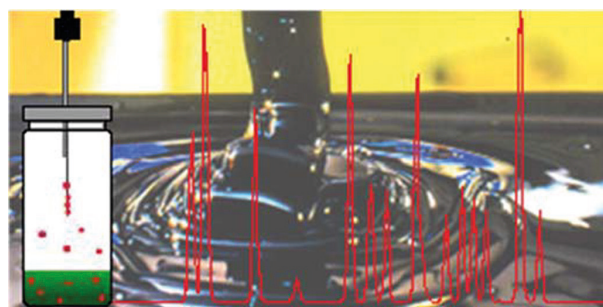
The radium present in the soil decays originating ^{222}Rn , a gas with high mobility that diffuses to the surface through pores, fissures in the soil and by the groundwater.

**2586 Evaluation of Benzene Derivatives Migration from Solid Residuals by Alternative Leaching Process Using HS-SPME GC-MS**

Jocinei Dognini and Luiz A. S. Madureira

Graphical Abstract

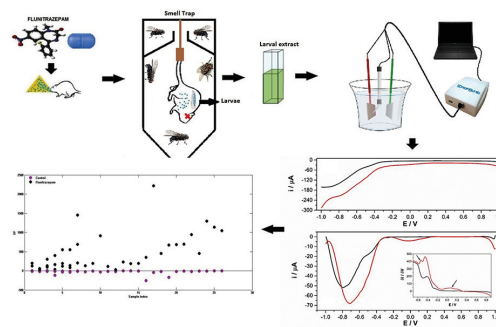
Alternative leaching process for the determination of benzene derivatives in petrochemical waste using headspace solid-phase micro-extraction gas chromatography-mass spectrometry (HS-SPME GC-MS).

**2595 Identification Using Classification Analysis of Flunitrazepam in Necrophagous Larvae via Differential Pulse Voltammetry and Fluorescence Excitation-Emission Matrix (EEM) Spectroscopy**

Leomir A. S. de Lima, Camilo L. M. Morais, Jéssica T. Jales,
Renata A. Gama, Sherlan G. Lemos and Kássio M. G. Lima

Graphical Abstract

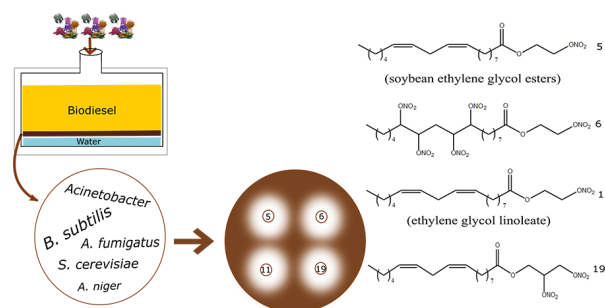
Experimental procedure to obtain samples of fly larvae extract and subsequent analysis by differential pulse voltammetry with E / V vs. Ag/AgCl reference electrode and molecular fluorescence spectroscopy.

**2605 Synthesis and Evaluation of Biocide and Cetane Number Improver Additives for Biodiesel from Chemical Changes in Triacylglycerides**

Kênia P. Costa, Stella F. do Valle, Thayana F. L. dos Santos,
Ellen T. Rangel, Angelo C. Pinto, Paulo A. Z. Suarez and
Michelle J. C. Rezende

Graphical Abstract

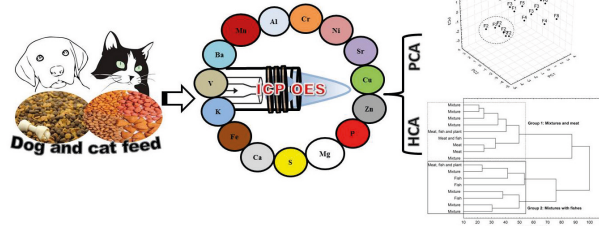
Biocide candidates from chemical transformations in triacylglycerides were evaluated against microorganisms which have been isolated from biodiesel/diesel blends. Four nitrated derivatives presented fungicidal activity.



2616 Evaluation of the Chemical Composition of Dry Feeds for Dogs and Cats

Silvânio S. L. Costa, Ana C. L. Pereira, Elisângela A. Passos,
SI online José P. H. Alves, Carlos A. B. Garcia and Rennan G. O. Araújo

Pattern recognition

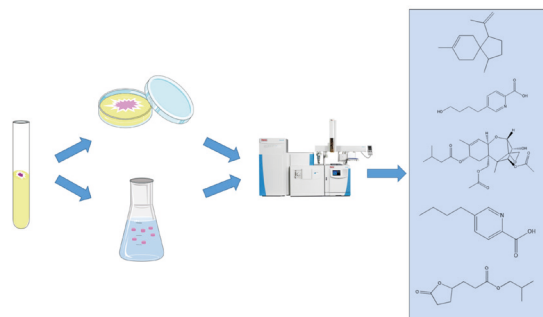


Graphical Abstract

In this work, the mineral composition of dry feeds for cat and dog was determined and evaluated according to regulatory agencies.

2626 Identification of *Fusarium oxysporum* Fungus in Wheat Based on Chemical Markers and Qualitative GC-MS Test

Carlos E. R. Senes, Nayara C. Saldan, Willian F. Costa,
SI online Terezinha I. E. Svidzinski and Cláudio C. Oliveira

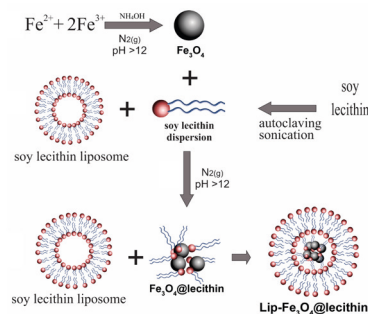


Graphical Abstract

Fusarium oxysporum was cultivated in liquid and solid culture media. Using gas chromatography coupled to mass spectrometry (GC-MS), it was possible to identify secondary metabolites from liquid and solid culture media that can be used as chemical markers for this fungus.

2636 Preparation of Magnetoliposomes with a Green, Low-Cost, Fast and Scalable Methodology and Activity Study against *S. aureus* and *C. freundii* Bacterial Strains

Rosângela M. F. da Costa e Silva, Luciano R. S. Lara,
SI online Jorge L. López, Ângela L. Andrade, Junnia A. C. Oliveira, Jacqueline A. Takahashi, Henriete S. Vieira, Tulio Matencio, Humberto O. Stumpf and Rosana Z. Domingues

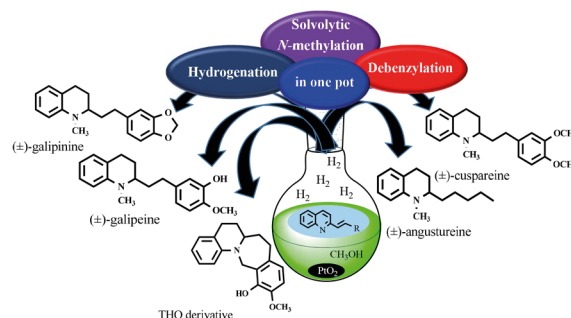


Graphical Abstract

A novel methodology, fast, low-cost and scalable, without the use of organic solvents and with the dual use of soy lecithin to prepare stable magnetoliposomes (MGLs).

2646 Unprecedented One-Pot Sequence for the Synthesis of Tetrahydroquinoline Alkaloids and Preliminary Evaluation of their Antibacterial Activity

Gaspar Diaz-Muñoz, Izabel L. Miranda, Suélen K. Sartori,
SI online Gabriel N. S. Dias, Markus Kohlhoff, Gislaine A. Purgato and Marisa A. N. Diaz



Graphical Abstract

A novel one-pot sequence (in 2 or 3 steps) was developed for the synthesis of the tetrahydroquinoline alkaloids (±)-galipinine, (±)-cuspareine, (±)-galipeine and (±)-angustureine, and the derivative (±)-11-methoxy-5,6,6a,7,8,13-hexahydro-13a-aza-benzo[5,6]cyclohepta[1,2-a]naphthalene-12-ol from their respective Wittig adducts.

Short Report

2657 Potential Antileishmanial Activity of 4-*N*-Acylhydrazone Pyrazolo[3,4-*d*]pyridazin-7-ones: Synthesis, *in vitro* Biological Evaluations and Computational Studies



SI online

Andrey P. Jacomini, Michael J. V. da Silva, Julia Poletto, Gessica M. Ribeiro, Jessica T. C. Yokoyama, Danielle L. Bidóia, Fávero R. Paula, Celso V. Nakamura, Maria Helena Sarragiotto and Fernanda A. Rosa

Graphical Abstract

Synthesis of new series of pyrazolo[3,4-*d*]pyridazin-7-ones with antileishmanial activity and low toxicity against *Leishmania amazonensis* (strain WHOM/BR/75/JOSEFA), promastigote and amastigote forms.

