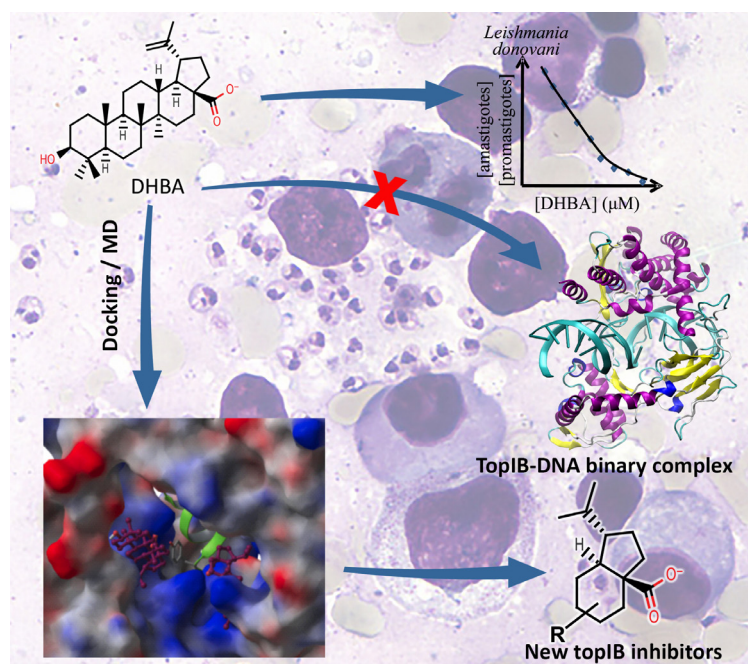


Cover Picture



Dihydrobetulinic acid (DHBA) is active against amastigotes and promastigotes from *Leishmania donovani* both *in vitro* and *in vivo* models. This compound inhibits the formation of the binary complex between topoisomerase IB (topIB) and DNA, and induces apoptosis. Based on docking and molecular dynamics studies we have identified the most probable binding site of DHBA on topIB. This computational model also revealed that a molecular fragment of this triterpenoid can be strategically relevant to develop new antileishmanial leads. Details are presented in the Article **The Octahydroindene Carboxyl Substructure from Dihydrobetulinic Acid is Essential to Inhibit Topoisomerase IB from *Leishmania donovani*** by Camila A. Rocha, Paulo R. S. Sanches, Reinaldo Marchetto and Aderson Zottis on page 591.

Contents

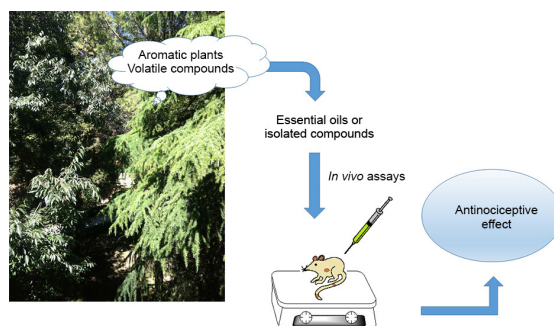
Review

435 Antinociceptive Effect of Essential Oils and Their Constituents: an Update Review

Eder J. Lenardão, Lucielli Savegnago, Raquel G. Jacob, Francine N. Victoria and Débora M. Martinez

Graphical Abstract

Plant essential oils (EOs) have been used for centuries in folk medicine to treat diverse disorders, including as analgesic to pain relief. This review covers the literature on the antinociceptive activity of EOs and their constituents from 2000 to 2015. The concepts involved in the nociception, the major clinical treatments used to treat pain and the main tests used to access the analgesic effect of natural compounds are discussed



Articles

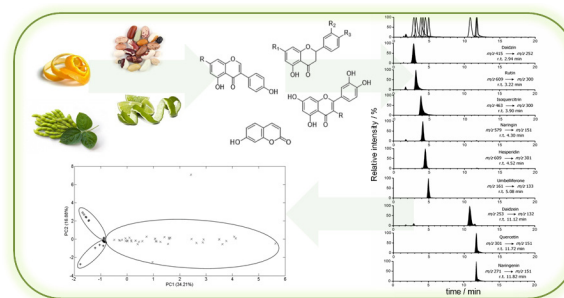
475 Application of a Quantitative HPLC-ESI-MS/MS Method for Flavonoids in Different Vegetables Matrices

Bruno Perlatti, João B. Fernandes, Maria F. G. F. Silva, Jorge A. Ardila, Renato L. Carneiro, Bruno H. S. Souza, Eduardo N. Costa, Wellington I. Eduardo, Arlindo L. Boiça Junior and Moacir R. Forim

SI online

Graphical Abstract

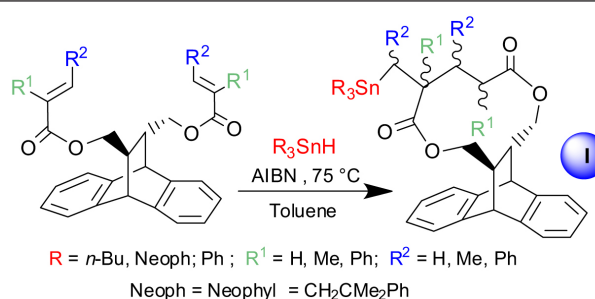
Different vegetable matrices were evaluated and discriminated by quantitative analysis of specific flavonoids using high-performance liquid chromatography coupled to electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS) and principal component analysis (PCA)



484 Synthesis of Organotin Substituted Tricyclic Macrodiolides

Flavia C. Zacconi, Romina A. Ocampo, Julio C. Podestá and Liliana C. Koll

SI online



Graphical Abstract

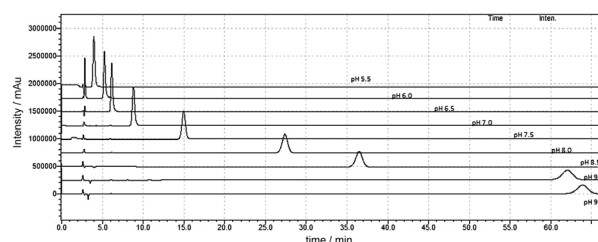
Synthesis of organotin substituted 11 membered macrocycles

493 Effect of Organic Solvent Composition on Dissociation Constants of Some Reversible Acetylcholinesterase Inhibitors

Y. Doğan Daldal, Ebru Çubuk Demiralay and Sibel A. Özkan

Graphical Abstract

Variation of the mobile phase pH is a key parameter to enhance the chromatographic selectivity and retention time for ionization compounds. Solvent effect was investigated for the developed method. Dissociation constant values were calculated by different percentages of acetonitrile/methanol in the mobile phase at different pH environment. This work can be used for drug discovery of acetylcholinesterase inhibitors



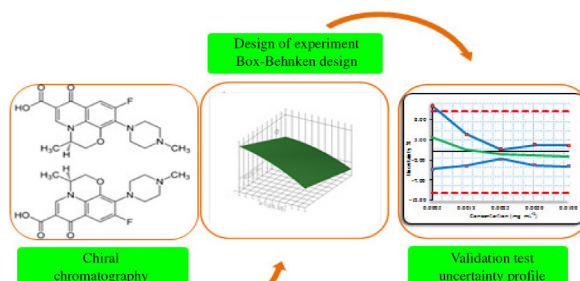
500 Application of a New Strategy of Validation Based on “β,γ-Content Tolerance Interval” for Checking the Chiral Chromatography Method for Quantification of the Chiral Impurity of Levofloxacin

Houda Bouchafra, Miloud El karbane, Mohamed Azougagh, Fayssal Jhilar, Saad Alawi Sosse, EL Mestafa El hadrami, Taoufiq Saffaj and Bouchaib Ihssane

SI online

Graphical Abstract

In order to get a chromatographic method able to yield a good separation, identification and quantification of the enantiomers (Levofloxacin and its (R)-enantiomer), chemometric tools should be appropriately applied, especially by applying the experimental designs methodology. In addition, in order to verify the optimized method we propose an innovative approach, recently developed in our laboratory called the uncertainty profile



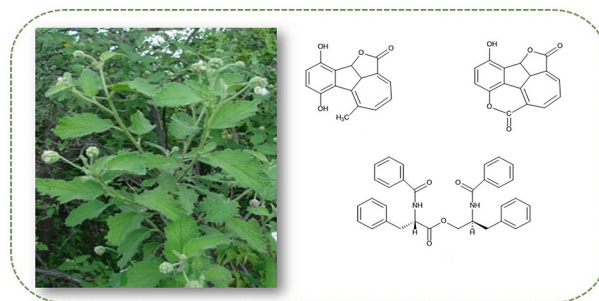
510 Meroterpenoid Hydroquinones from *Cordia globosa*

Ana Karine O. Silva, André Luis L. de Oliveira, Francisco das Chagas L. Pinto, Karisia S. B. de Lima, Raimundo Braz-Filho, Edilberto R. Silveira and Otilia Deusdênia L. Pessoa

SI online

Graphical Abstract

Two new meroterpenoid hydroquinones along with the known peptide (S)-N-benzoylphenylalanine-(S)-2-benzamide-3-phenylpropyl ester were isolated from the roots of *Cordia globosa*. Their structures were determined by 1D and 2D nuclear magnetic resonance (NMR) spectrometry, Fourier transform infrared (FTIR) spectroscopy and high resolution atmospheric pressure chemical ionization mass spectrometry (HRAPCIMS)

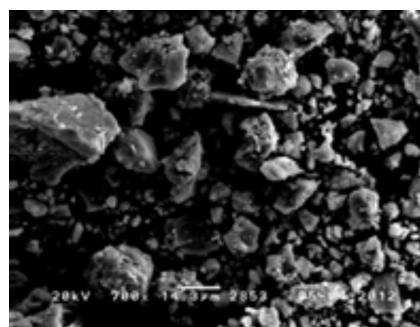
**515 Cr/Al Oxide as Solid Acid Catalyst to Afford Babassu Biodiesel**

Carla V. R. Moura, Haroldo L. S. Neres, Mariane G. Lima, Edmilson M. Moura, Jose M. Moita Neto, José E. de Oliveira, José R. O. Lima, Ilza M. Stolin and Eugênio C. E. Araújo

SI online

Graphical Abstract

Solid acid catalyst was obtained by the mixture of Al/Cr oxides to afford babassu biodiesel with a great acidity 5.0%. The yield of biodiesel was about 97.5% in 15 h and 70 °C

**526 Alternative Igniters Based on Oxidant Salts for Microwave-Induced Combustion Method**

Leticia S. F. Pereira, Gabrielle D. Iop, Mariele S. Nascimento, Liange O. Diehl, Cezar A. Bizzi, Juliano S. Barin and Erico M. M. Flores

Graphical Abstract

Use of solutions of oxidant salts as igniters, understanding the ignition assisted by microwaves, and the use of alternative igniters for microwave-induced combustion for further metals determination

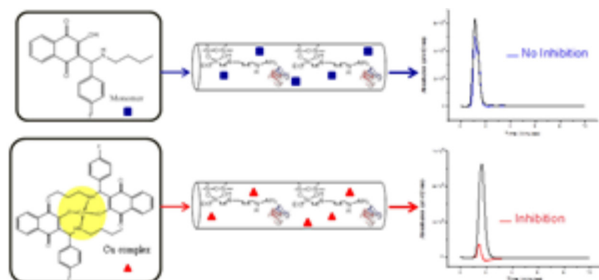
**534 Aminonaphthoquinone Mannich Bases Derived from Lawsone and Their Copper(II) Complex Derivatives: Synthesis and Potential Cholinesterase Inhibitors as Identified by On-flow Assay**

Adriana F. L. Vilela, Bárbara M. Frugeri, André L. F. Sarria, Rodrigo O. S. Kitamura, João B. Fernandes, Maria F. G. F. Silva, Quezia B. Cass and Carmen L. Cardoso

SI online

Graphical Abstract

A new series of Mannich bases and their Cu²⁺ complexes were synthesized and evaluated for their potential as selective cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BChE)] inhibitors by on-flow assay. All copper complexes were more active than the Mannich bases

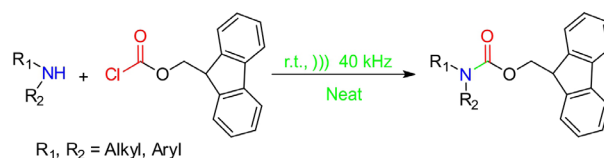


546 A Greener, Efficient and Catalyst-Free Ultrasonic-Assisted

Protocol for the *N*-Fmoc Protection of Amines

SI online

Rachida Mansouri, Zineb Aouf, Salah Lakrouf,
Malika Berredjem and Nour-Eddine Aouf



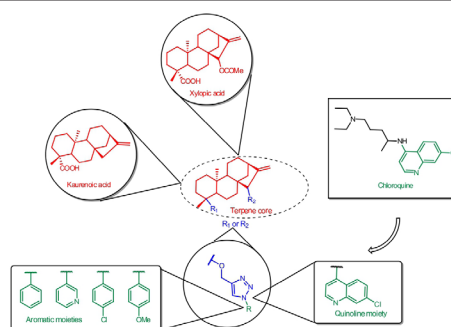
Graphical Abstract

An eco-sustainable ultrasound-assisted method for the *N*-Fmoc protection is reported. Mildness, efficiency, excellent yielding and short reaction times are the main advantages of this new protocol

551 Synthesis, *in vitro* Antimalarial Activity and *in silico* Studies of Hybrid Kauranoid 1,2,3-Triazoles Derived from Naturally Occurring Diterpenes

SI online

Juliana de O. Santos, Guilherme R. Pereira, Geraldo C. Brandão, Tatiane F. Borgati, Lucas M. Arantes, Renata C. de Paula, Luciana F. Soares, Maria F. A. do Nascimento, Márlia R. C. Ferreira, Alex G. Taranto, Fernando P. Varotti and Alaíde B. de Oliveira

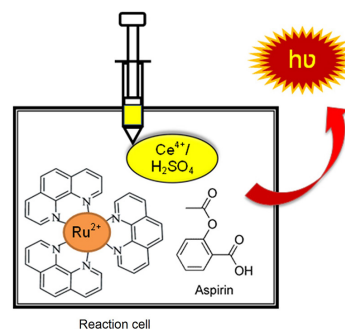


Graphical Abstract

The kauranoid moieties core in the novel 1,2,3-triazole-1,4-disubstituted hybrid molecules were synthesized by copper-catalyzed azide-alkyne cycloaddition (CuAAC) reactions. All compounds were evaluated for antiplasmodial and cytotoxic activity

566 Determination of Aspirin Using Chemiluminescence System of Tris(1,10 phenanthroline)Ruthenium(II)-Cerium(IV)

Ali Mokhtari, Mohsen Keyvanfard, Iraj Emami, Nastaran J. Delouei, Hatameh F. Pishkhani, Aida Ebrahimi and Hossein Karimian

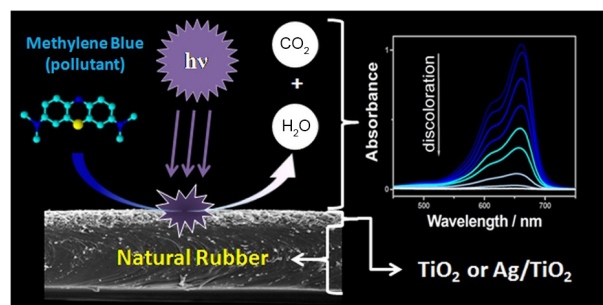


Graphical Abstract

A chemiluminescence method based on the enhancement effect of aspirin in the system of tris(1,10 phenanthroline)ruthenium(II), with acidic Ce^{IV} has been proposed

575 Use of Natural Rubber Membranes as Support for Powder TiO_2 and Ag/TiO_2 Photocatalysts

Jusinei M. Stropa, Aline S. Herrero, Silvio C. Oliveira, Alberto A. Cavaleiro, Renato F. Dantas, Samuel L. Oliveira, Amílcar Machulek Jr. and Lincoln C. S. Oliveira



Graphical Abstract

Methylene blue discoloration on a natural rubber membrane surface containing TiO_2 or Ag/TiO_2 . On ultraviolet-visible (UV-Vis) spectrophotometric analysis, decreased absorbance intensity indicates methylene blue degradation

- 584 **Pressurized Flow Solubilization System Using Electromagnetic Induction Heating Technique for Simultaneous Determination of Inorganic Elements (Ba, Ca, Cd, Cu, Fe, Mg, Mn, Na, Pb, Sr, Zn) in Sonicate Slurries of Biological Materials by Microwave Induced Plasma Optical Emission Spectrometry (MIP-OES)**
Henryk Matusiewicz and Mariusz Ślachciński



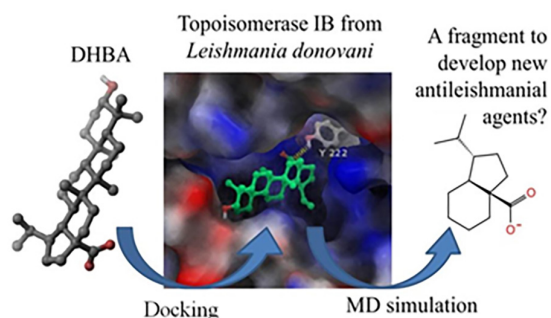
Graphical Abstract

Pressure electromagnetic induction heating flow solubilization system

- 591 **The Octahydroindene Carboxyl Substructure from Dihydrobetulinic Acid is Essential to Inhibit Topoisomerase IB from *Leishmania donovani***
Camila A. Rocha, Paulo R. S. Sanches, Reinaldo Marchetto and Aderson Zottis

Graphical Abstract

Dihydrobetulinic acid is a competitive inhibitor of topoisomerase IB from *Leishmania donovani*. By docking and simulations of molecular dynamics it was identified a potential fragment to develop new antileishmanial compounds



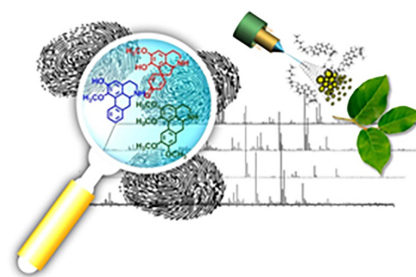
- 599 **Chemotaxonomy of the Amazonian *Unonopsis* Species Based on Leaf Alkaloid Fingerprint Direct Infusion ESI-MS and Chemometric Analysis**

SI online

Felipe M. A. Silva, Francinaldo A. Silva Filho, Bruna R. Lima, Richardson A. Almeida, Elzalina R. Soares, Hector H. F. Koolen, Afonso D. L. Souza and Maria L. B. Pinheiro

Graphical Abstract

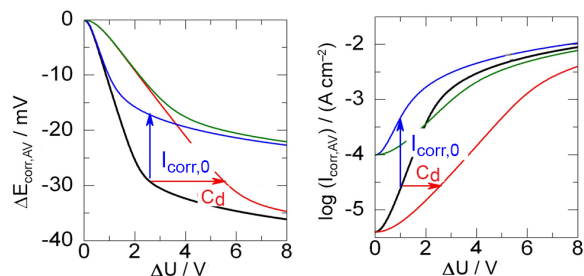
Alkaloid fingerprint along with multivariate analysis provided a simple and effective approach to differentiate Amazonian *Unonopsis* species



- 605 **AC Induced Corrosion of Underground Steel Pipelines. Faradaic Rectification under Cathodic Protection: II. Theoretical Approach with Electrolyte Resistance and Double Layer Capacitance for Bi-Tafelian Corrosion Mechanism**
Ibrahim Ibrahim, Michel Meyer, Hisasi Takenouti and Bernard Tribollet

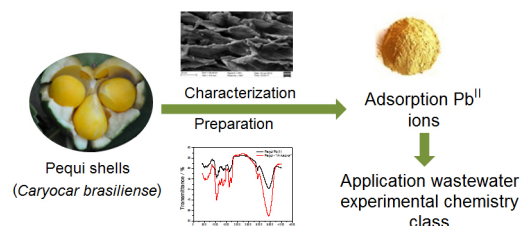
Graphical Abstract

Effect of the AC stray voltage on the faradaic rectification by the double layer capacitance and the corrosion current density



616 Characterization of Pequi (*Caryocar brasiliense*) Shells and Evaluation of Their Potential for the Adsorption of Pb^{II} Ions in Aqueous Systems

Dayane J. Amorim, Hélen C. Rezende, Érica L. Oliveira, Ione L. S. Almeida, Nívia M. M. Coelho, Túlio N. Matos and Cleide S. T. Araújo

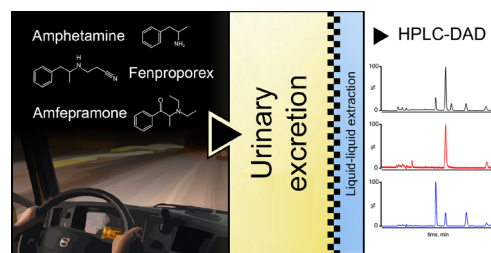


Graphical Abstract

Pequi (*Caryocar brasiliense*) shells were characterized by point of zero charge (PZC), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy-energy dispersive spectroscopy (SEM-EDS) and the adsorbent material was studied for Pb^{II} ions adsorption

624 Determination of Amphetamine, Amfepramone and Fenproporex in Urine Samples by HPLC-DAD: Application to a Population of Brazilian Truck Drivers

Juliana Takitane, Rafael M. Almeida, Tiago F. Oliveira, Natanael V. Prado, Daniel R. Muñoz, Vilma Leyton and Mauricio Yonamine



Graphical Abstract

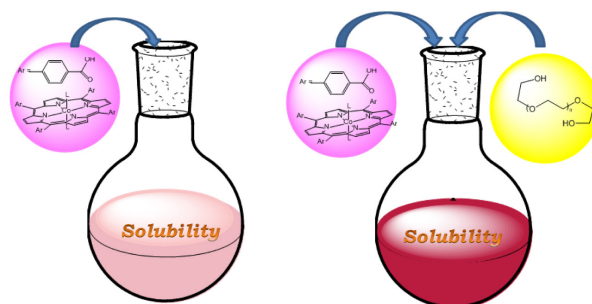
Liquid-liquid extraction was applied in urine samples collected from truck drivers for the determination of amphetamines by high performance liquid chromatography with diode array detection (HPLC-DAD)

Short Report

631 Effect of Polyethyleneglycols (PEG) on Solubility of Co^{III} 5,10,15,20-Tetra(4-carboxyphenyl)porphyrin and Methylimidazolyl Axial Complex at 298.2 K: Experiment and Modeling

SI online

Tatyana V. Volkova, Vasiliy A. Golubev, Mikhail Y. Nikiforov, Galina M. Mamardashvili, Nugzar Z. Mamardashvili and German L. Perlovich



Graphical Abstract

In this study simple and efficient method of enhancing the solubility of Co^{III} porphyrins based on polyethyleneglycol additions to water solution was proposed

Additions and Corrections

639 Equilibrium and Out-Of-Equilibrium Investigation of Proton Exchange and Cu^{II} and Zn^{II} Complexation on Fungal Mycelium (*Trametes hirsuta*)

Vicente R. Almeida, Bruno Szpoganicz, Lei Chou, Kitty Baert, Annick Hubin and Steeve Bonneville