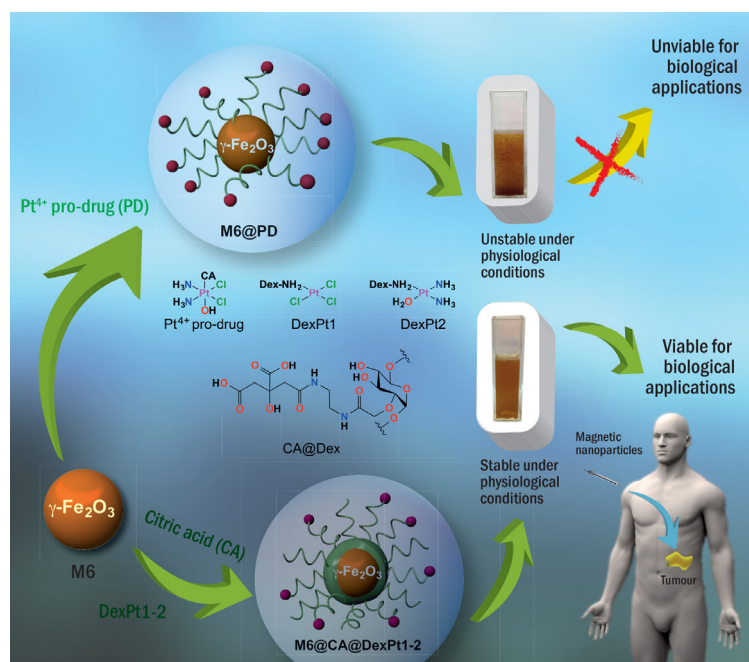


Cover Picture



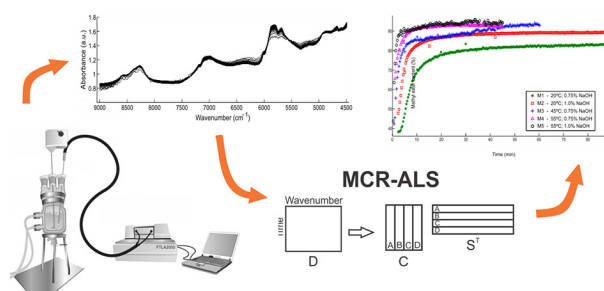
In this paper we describe synthetic strategies for improving the colloidal properties of platinum drug-functionalized superparamagnetic iron oxide nanoparticles (SPIONs). Protecting the surface of SPIONs with citric acid and further functionalization with Pt^{2+} complexes modified dextran is an excellent tactic to obtain stable magnetic nanoparticles under physiological conditions. Details are presented in the Article **Studies of the Colloidal Properties of Superparamagnetic Iron Oxide Nanoparticles Functionalized with Platinum Complexes in Aqueous and PBS Buffer Media** by *Gustavo B. da Silva, Marzia Marciello, María del Puerto Morales, Carlos J. Serna, Maria D. Vargas, Célia M. Ronconi and Rocío Costo* on page 731.

Contents

Articles

- 695** NIR Monitoring and Modelling of Soybean Oil Methanolysis with Multivariate Curve Resolution-Alternating Least Squares with Correlation Constraint
Rafaella F. Sales, Suzana M. de Lima, Luiz Stragevitch, Maria Fernanda Pimentel and Anna de Juan

Graphical Abstract
 NIR monitoring of transesterification reactions and application of MCR-ALS with correlation constraint to estimate methyl ester concentration profiles.



707 Chemical Constituents of *Psychotria nemorosa* Gardner and Antinociceptive Activity

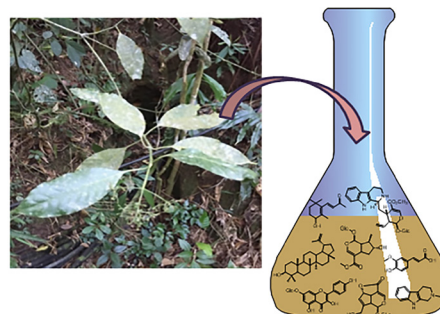


SI online

Nívea O. Calixto, Millena S. Cordeiro, Thais B. S. Giorno, Gibson G. Oliveira, Norberto P. Lopes, Patricia D. Fernandes, Angelo C. Pinto and Claudia M. Rezende

Graphical Abstract

This is the first phytochemical study of *Psychotria nemorosa* Gardner leaves (Rubiaceae) established in a metabolomic perspective by GC-MS and LC-MS, besides its antinociceptive activity.

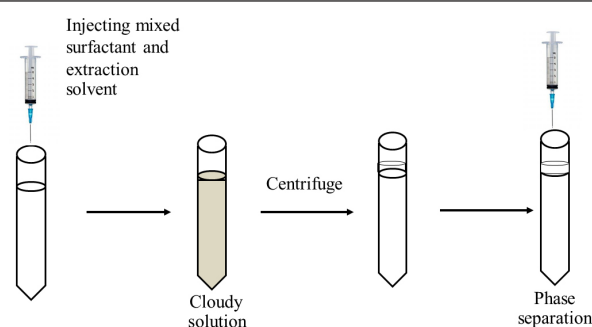


724 Cationic Micellar Precipitation for Simultaneous Preconcentration of Benzimidazole Anthelmintics in Milk Samples by High-Performance Liquid Chromatography

Jitlada Vichapong, Yanawath Santaladchaiyakit, Supalax Srijaranai and Rodjana Burakham

Graphical Abstract

Micellar precipitation process was investigated. This method provides high efficacy for extraction of benzimidazoles analysis.



731 Studies of the Colloidal Properties of Superparamagnetic Iron Oxide Nanoparticles Functionalized with Platinum Complexes in Aqueous and PBS Buffer Media

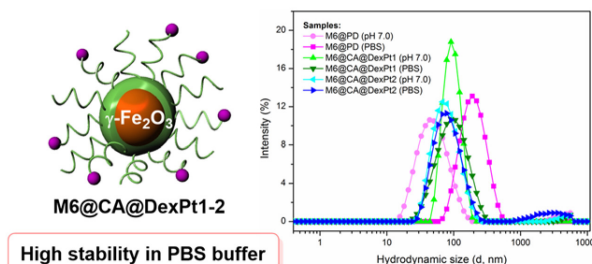


SI online

Gustavo B. da Silva, Marzia Marciello, María del Puerto Morales, Carlos J. Serna, Maria D. Vargas, Célia M. Ronconi and Rocío Costo

Graphical Abstract

Novel dextran-coated SPIONs functionalized with platinum complexes afford high colloidal stability in aqueous and PBS buffer media.

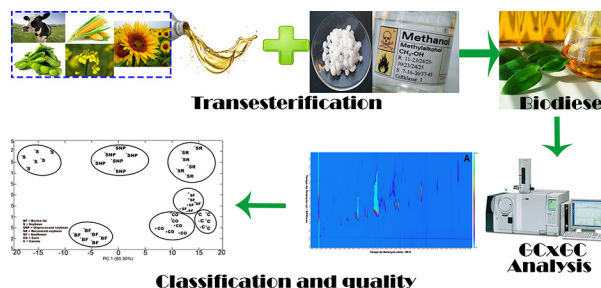


740 Exploratory Analysis of Biodiesel by Combining Comprehensive Two-Dimensional Gas Chromatography and Multiway Principal Component Analysis

Noroska G. S. Mogollón, Fabiana A. L. Ribeiro, Ronei J. Poppi, Araceli L. Quintana, Juan A. G. Chávez, Darwin A. P. Agualongo, Helga G. Aleme and Fabio Augusto

Graphical Abstract

The synthesis of biodiesel requires analysis with high resolution and detectability for determining the biodiesel raw material.

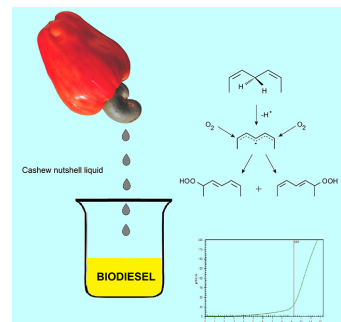


747 The Use of the Liquid from Cashew Nut Shells as an Antioxidant in Biodiesel

Flavio A. Bastos and Matthieu Tubino

Graphical Abstract

Cashew nutshell liquid (CNSL) can be used as antioxidant in biodiesel increasing its oxidative stability, even when added in 0.1% m/m or in lower concentration.

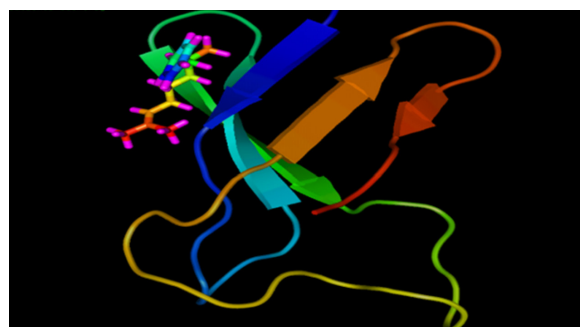


756 Synthesis, Characterization and Antimicrobial Activities of Copper, Nickel, Cobalt, Chromium Complexes Derived from (Z)-4-Fluoro-N-(2,7-dimethylhept-6-enylidene)benzenamine

Sridhar.G, Mohammed Bilal.I, Easwaramoorthy.D, Kutti Rani.S, Siva Kumar.B and Chelli Sai Manohar

Graphical Abstract

We obtained novel binuclear chromium(III)-ligand bridging complex. The docking study of the Schiff base ligand illustrates the binding interactions with PAF protein.



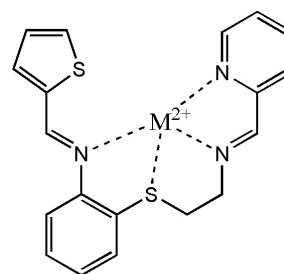
768 Synthesis and Characterization of a New Unsymmetrical Potentially Pentadentate Schiff Base Ligand and Related Complexes with Manganese(II), Nickel(II), Copper(II), Zinc(II) and Cadmium(II)

SI online

Ahmad Ali Dehghani-Firouzabadi and Sakineh Firouzmandi

Graphical Abstract

New unsymmetric thioether Schiff base amine, unsymmetric Schiff base ligand (L) and related complexes of this ligand were prepared and characterized by the appropriate spectroscopic methods.



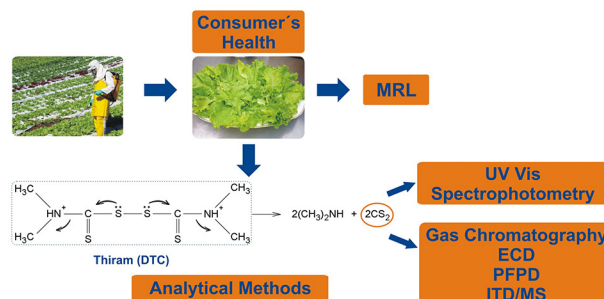
M = Mn, Ni, Cu, Zn, Cd

775 Comparison Between Three Chromatographic (GC-ECD, GC-PFPD and GC-ITD-MS) Methods and a UV-Vis Spectrophotometric Method for the Determination of Dithiocarbamates in Lettuce

Ionara R. Pizzutti, André de Kok, Rosselei C. da Silva and Graciele N. Rohers

Graphical Abstract

Lettuce is an important crop consumed in Brazil and dithiocarbamates are the most frequently fungicides detected in Brazilian monitoring programs. Due to this, it is necessary analytical methods with high quality in order to determine dithiocarbamates residues in lettuce.

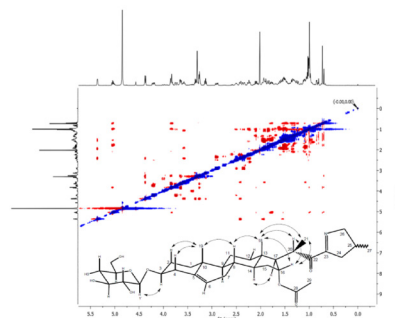


782 Three New Steroidal Glycoalkaloids from *Solanum pseudoquina* A. St.-Hil. (Solanaceae)

Vitor Soares, Thaís A. Bezerra, Rita C. A. Lafetá,
SI online Ricardo M. Borges and Antonio Jorge R. da Silva

Graphical Abstract

Rotating frame nuclear Overhauser effect spectroscopy (ROESY) correlations were used in the elucidation of the overall stereochemistry of the three alkaloids obtained from *S. pseudoquina* A. St.-Hil.

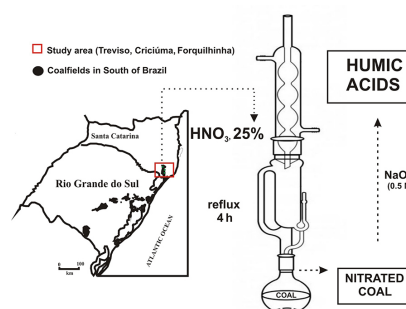


790 Impact of HNO_3 Solution Treatment of South Brazil Coal Matrices on Their Chemical Composition and Humic Acids Yield

Deborah P. Dick, Janaina B. da Costa, Anderson José B. Leite
and Eduardo A. Brocchi

Graphical Abstract

This study demonstrated that the nitration of coal tailings to increase humic acids yield is a promising alternative for a sustainable fate of these residues.

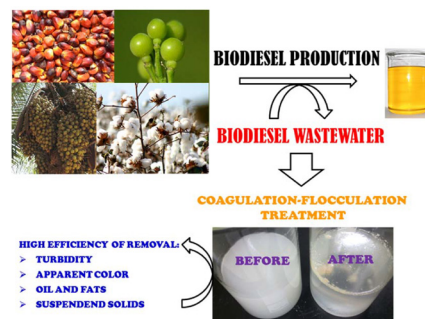


800 Biodiesel Wastewater Treatment by Coagulation-Flocculation: Evaluation and Optimization of Operational Parameters

Bárbara R. Gonçalves, Waldomiro Borges Neto,
SI online Antonio E. H. Machado and Alam G. Trovó

Graphical Abstract

A coagulation-flocculation process was evaluated as alternative for treatment of biodiesel wastewater, being obtained efficiencies between 82 and 99% for removal of apparent color, oils and fats, turbidity and suspended solids.

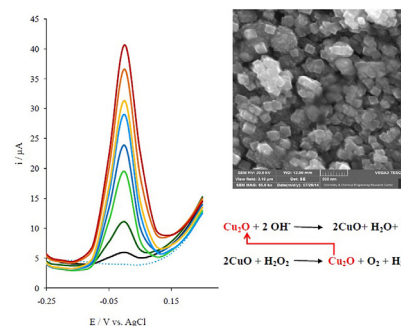


808 Low Potential and Non-Enzymatic Hydrogen Peroxide Sensor Based on Copper Oxide Nanoparticle on Activated Pencil Graphite Electrode

SI online Mohammad Ali Kamyabi and Nasim Hajari

Graphical Abstract

Chemically activated pencil graphite electrode modified with CuO nanocubes presented as electrochemical H_2O_2 sensor. The presented sensor has excellent electrocatalytic activity toward H_2O_2 oxidation (dramatically decrease in H_2O_2 oxidation overpotential, at about +0.05 V vs. Ag/AgCl).

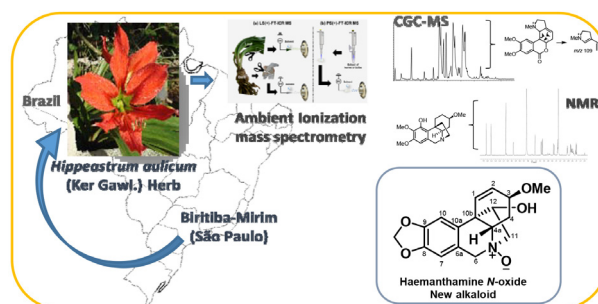


819 Identification of Alkaloids from *Hippeastrum aulicum* (Ker Gawl.) Herb. (Amaryllidaceae) Using CGC-MS and Ambient Ionization Mass Spectrometry (PS-MS and LS-MS)

SI online *Carlani D. P. B. Bessa, Jean P. de Andrade, Renata S. de Oliveira, Eloilson Domingos, Heloia Santos, Wanderson Romão, Jaume Bastida and Warley S. Borges*

Graphical Abstract

Typical Amaryllidaceae alkaloids have been identified from *Hippeastrum aulicum* by means of capillary gas chromatography-mass spectrometry (CGC-MS). Leaf and paper spray mass spectrometry were carried out and the results obtained were in agreement with CGC-MS data. NMR data for the new compound haemanthamine *N*-oxide are also reported.

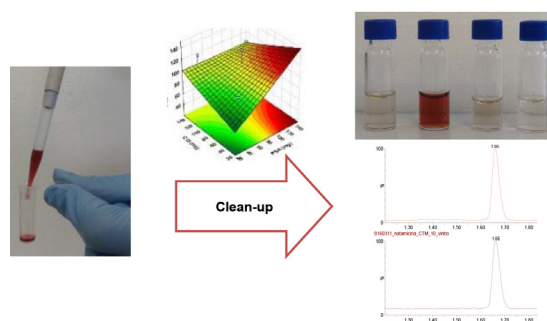


831 Fast Sample Preparation Method Using Ultra-High Performance Liquid Chromatography Coupled to Tandem Mass Spectrometry for Natamycin Determination in Wine Samples

SI online *Gabrieli Bernardi, Tiele M. Rizzetti, Martha B. Adaime, Renato Zanella and Osmar D. Prestes*

Graphical Abstract

In this work a fast and efficient method was optimized by central composite design, validated and applied for natamycin residues determination in wine samples by UHPLC-MS/MS.

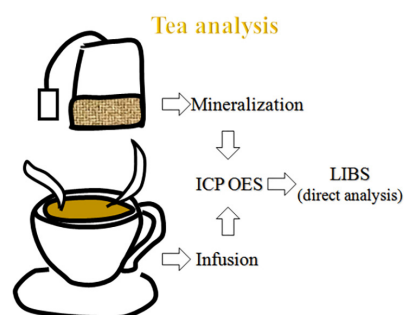


838 Comparison of ICP OES and LIBS Analysis of Medicinal Herbs Rich in Flavonoids from Eastern Europe

Daniel F. Andrade, Edenir Rodrigues Pereira-Filho and Pawel Konieczynski

Graphical Abstract

Spectroanalytical analysis of tea samples using ICP OES (infusion and mineralization) and direct Ca, K and Mg determination using LIBS

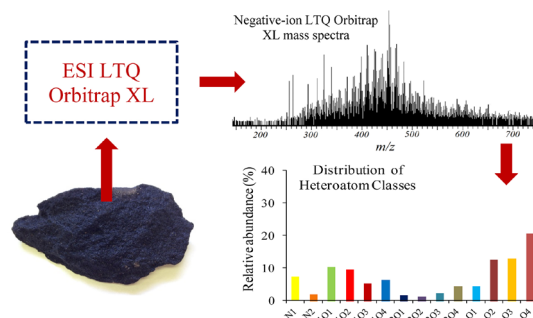


848 Characterization of Acidic Compounds in Brazilian Tar Sand Bitumens by LTQ Orbitrap XL: Assessing Biodegradation Using Petroleomics

Laercio L. Martins, Célio Fernando F. Angolini, Georgiana F. da Cruz and Anita J. Marsaioli

Graphical Abstract

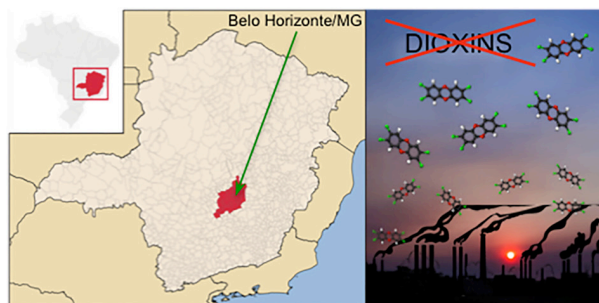
The acidic fraction of tar sand bitumens from Pirambóia Formation, Paraná Basin, were analyzed by negative-ion ESI LTQ Orbitrap XL. The distribution of heteroatom classes determined by the obtained mass spectra was used to assess biodegradation.



858 PCDD/Fs and PCBs in Soils: a Study of Case in the City of Belo Horizonte-MG

Igor C. Pussente, Guillaume ten Dam, Stefan van Leeuwen and Rodinei Augusti

SI online

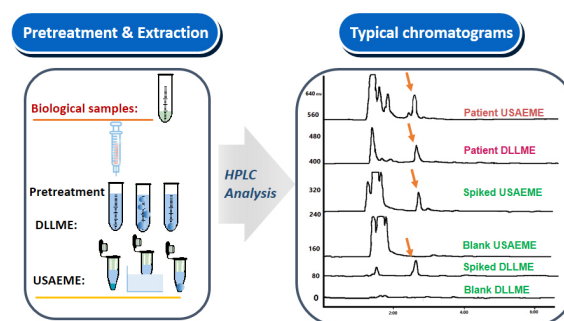


Graphical Abstract

Levels of polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans (PCDD/Fs) and polychlorinated biphenyls (PCBs) were investigated in soils from Belo Horizonte-MG.

868 Development and Validation of Ultrasound Assisted and Dispersive Liquid-Liquid Microextractions Combined with HPLC-UV Method for Determination of Bosentan in Human Plasma and Urine

Sanaz Sajedi-Amin, Karim Asadpour-Zeynali, Maryam Khoubnasabjafari, Farid Rashidi and Abolghasem Jouyban

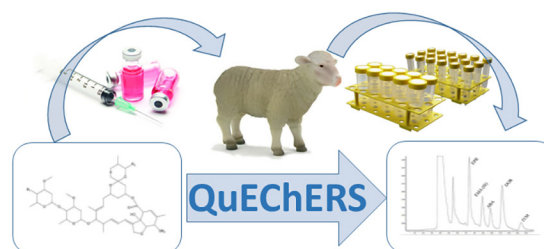


Graphical Abstract

Liquid-liquid microextraction methods (DLLME and USAEME) combined with LC-UV for determination of bosentan in biological samples.

878 Evaluation of QuEChERS Sample Preparation for Determination of Avermectins Residues in Ovine Muscle by HPLC-FD and UHPLC-MS/MS

Nelson M. G. Bandeira, Lucila C. Ribeiro, Tiele M. Rizzetti, Manoel L. Martins, Martha B. Adaime, Renato Zanella and Osmar D. Prestes

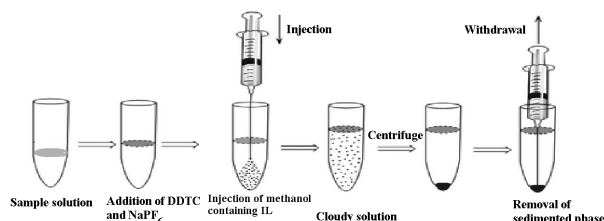


Graphical Abstract

The concern about the presence of veterinary drugs residues in food of animal origin has prompted the search for alternative methods able to detect low levels of these compounds in a simple and efficient way. Thus, in this work a QuEChERS method was successfully modified and validated for avermectins residues determination in ovine muscle samples by HPLC-FD and UHPLC-MS/MS.

887 Determination of Traces of Ni, Cu, and Zn in Wastewater and Alloy Samples by Flame-AAS after Ionic Liquid-Based Dispersive Liquid Phase Microextraction

Vahid Zare-Shahabadi, Parisa Asaadi, Fatemeh Abbasitabar and Abbas Shirmardi



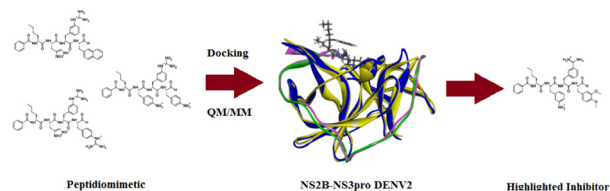
Graphical Abstract

To the sample solution, appropriate amounts of DDTC (complexing agent) and NaPF_6 were added. After standing for 2 min, 0.5 mL methanol containing 0.13 IL was injected rapidly. After centrifuging, extraction phase was mixed with 500 μL methanol prior to the flame-AAS analysis.

895 Docking and QM/MM Studies of NS2B-NS3pro Inhibitors: a Molecular Target against the Dengue Virus

Isabella P. Godói, William Gustavo Lima, Moacyr Comar Junior, Ricardo José Alves, Jaqueline Maria S. Ferreira, De-Xin Kong and Alex G. Taranto

SI online



Graphical Abstract

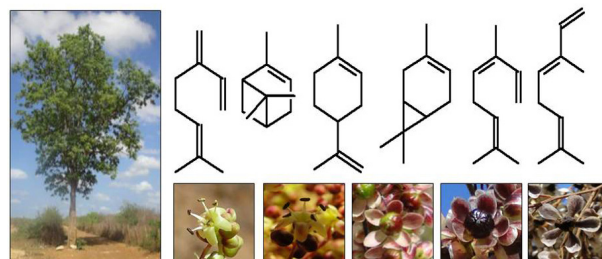
Peptidomimetics were considered as inhibitor candidates for NS2B-NS3pro DENV-2. Molecular docking and QM/MM calculations were used to evaluate these various compounds. Ligand Bz-Nle-m(Am)Phe-m(IIm)Phe-(dMo)Phe-H was found to be the best inhibitor candidate for this molecular template.

These findings may motivate additional virtual screening based on the pharmacophoric hypothesis to characterize lead compounds for therapies targeted against DENV.

907 Intraspecific Variation of the Volatile Chemical Composition of *Myracrodruon urundeuva* Fr. Allem. ("Aroeira-do-Sertão"): Characterization of Six Chemotypes

Nayara Coriolano de Aquino, Renata Mendonça Araújo and Edilberto Rocha Silveira

SI online



Graphical Abstract

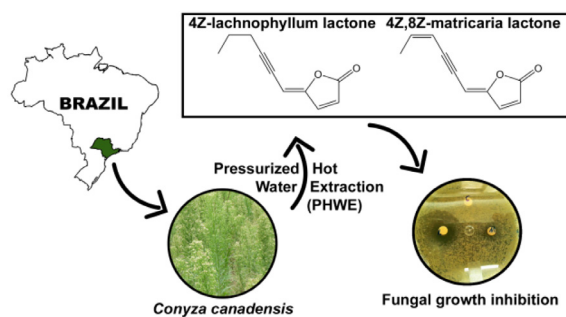
GC-MS and NMR analyzes of the essential oil from leaves of 62 individual specimens of *Myracrodruon urundeuva* ("aroeira-do-sertão") permitted to identify six different chemotypes characterized by the major constituents: myrcene, α -pinene, limonene, Δ^3 -carene, and (Z) and (E)- β -ocimene.

Short Reports

913 *Conyza canadensis*: Green Extraction Method of Bioactive Compounds and Evaluation of Their Antifungal Activity

Rafael S. Porto, Susanne Rath and Sonia C. N. Queiroz

SI online



Graphical Abstract

Compounds obtained from the plant *Conyza canadensis* through pressurized hot water extraction presented antifungal activity.

920 The Use of Near Infrared Spectroscopy and Multivariate Calibration for Determining the Active Principle of Olanzapine in a Pharmaceutical Formulation

Marcelo V. P. Amorim, Fernanda S. L. Costa, Cícero F. S. Araújo and Kássio M. G. Lima

Graphical Abstract

Active principle of olanzapine in different pharmaceutical excipients using near infrared spectroscopy (NIRS) and multivariate calibration was developed.

