

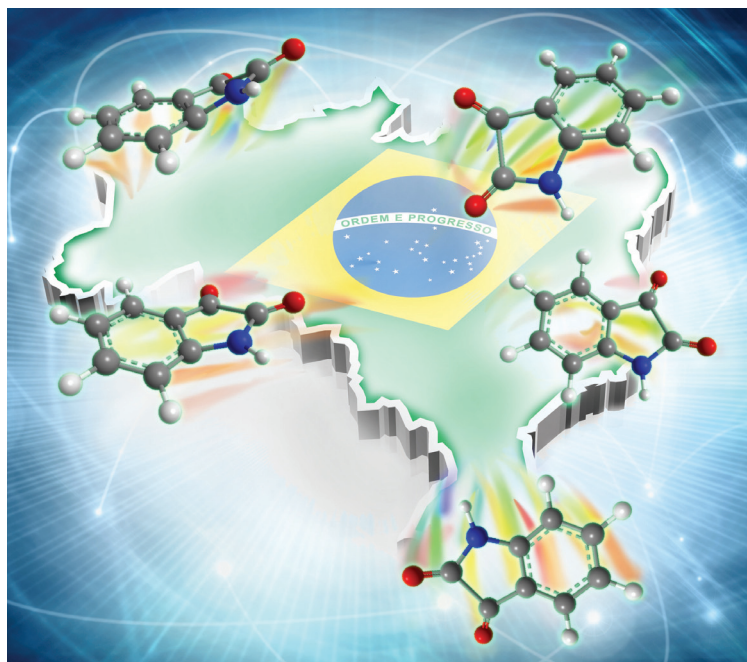
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Cover Picture



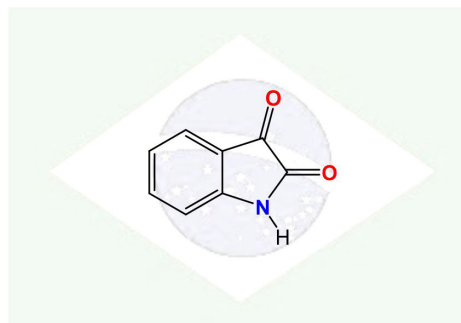
Isatin was synthesised in 1840 before it was discovered in the nature. Its derivatives are found in the parotid gland secretions of the Bufo frog, in the egg masses of the Australian mollusc *Dicathais orbita*, in plants of the *Isatis* genus and in the species *Couroupita guianensis*, Aubl, *Melochia tomentosa* and *Boronella koniamboensis*. It is an important raw material for the synthesis of a wide spectrum of bioactive compounds. Its derivatives exhibit antiviral, anti-inflammatory, anticonvulsant and antitumor activities, among others. This account discusses studies performed by several Brazilian research groups, including the investigations of its structural changes, the design of biological assays and some novel synthesis routes. Details are presented in the Account **Isatin, a Versatile Molecule: Studies in Brazil** by *Bárbara V. Silva* on page 707.

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Account

707 Isatin, a Versatile Molecule: Studies in Brazil

Bárbara V. Silva



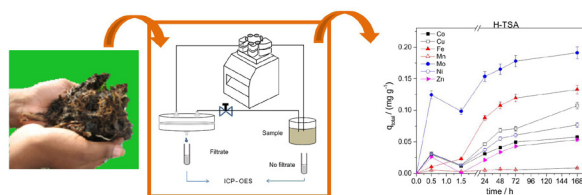
Graphical Abstract

Isatin is a small, versatile and widely applicable pharmacological molecule. Several Brazilian research groups have actively contributed to the development of novel synthetic routes to isatin derivatives, structural studies and the design of biological assays

Articles

721 Adsorption and Release of Micronutrients by Humic Extracted from Peat Samples

Danielle Goveia, Camila de A. Melo, Lilian K. de Oliveira, Leonardo F. Fraceto, Julio Cesar Rocha, Newton Luiz Dias Filho and André Henrique Rosa

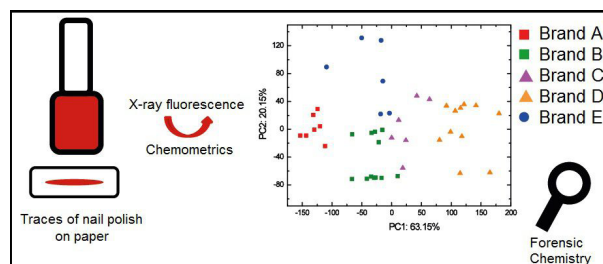


Graphical Abstract

Scheme of the analytical procedure used to determine the micronutrient adsorption/desorption capacity of humic extracted from peat samples. Conditions: ultrafiltration system (Sartorius Ultrasart X), 1 kDa polyethersulfone membrane (Gelman Pall-Filtron OMEGA)

731 Use of Portable X-ray Fluorescence to Discriminate Brands of Nail Polishes: a Potential Forensic Tool

Gustavo G. Shimamoto, Juliana Terra and Maria Izabel M. S. Bueno



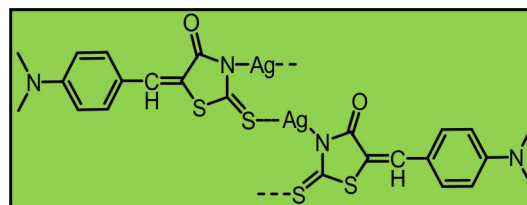
Graphical Abstract

The figure shows the steps for grouping nail polish samples depending on their brands to contribute as an useful evidence in forensic science. The proposed methodology is a quick, low cost and green alternative

736 FAAS Determination of Ag(I) in Water, Anode Slime, Rock and Cream Samples by Solid Phase Extraction Method based on Sepabeads SP207/5-(*p*-Dimethylaminobenzylidene) Rhodanine Combination

SI online

Emre Yavuz, Şerife Tokalioğlu and Serkan Şahan



Graphical Abstract

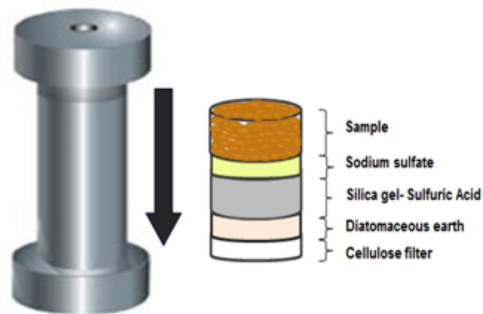
5-(*p*-Dimethylaminobenzylidene) rhodanine (PDR) is a derivative of rhodanine that is especially suitable as a sensitive and highly selective reagent for silver. It forms slightly soluble red precipitate with Ag(I)

743 Integrated Pressurized Solvent Extraction-Cleanup for the Rapid Determination of Polychlorinated Biphenyls in Meat Samples

Carla Toledo-Neira, Pedro Enríquez and Pablo Richter

Graphical Abstract

Integrated Pressurized liquid extraction (PLE) with solid phase extraction (SPE) cleanup method was developed for determination of polychlorinated biphenyls in chicken and pork meat samples. Extraction variables were optimized by experimental design and good analytical features were obtained

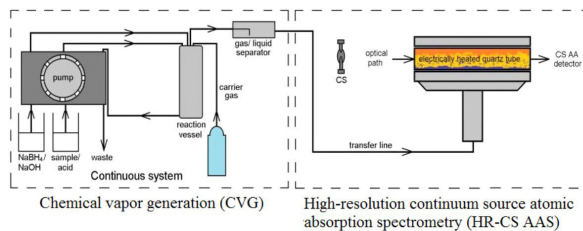


749 Determination of Gold by High-Resolution Continuum Source Atomic Absorption Spectrometry with Chemical Vapor Generation

Magdalena Krawczyk and Henryk Matusiewicz

Graphical Abstract

In this study, the analytical potential of chemical vapor generation (CVG) and high-resolution continuum source atomic absorption spectrometry (CVG HR-CS AAS) with quartz tube atomization in the determination of gold was evaluated

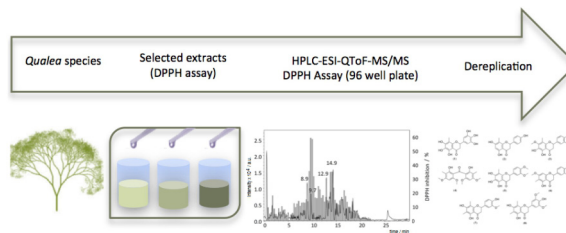


758 Dereplication of Phenolic Derivatives of *Qualea grandiflora* and *Qualea cordata* (Vochysiaceae) using Liquid Chromatography coupled with ESI-QToF-MS/MS

SI online Fausto Carnevale Neto, Cristian D. Siquitelli, Alan C. Pilon, Dulce H. S. Silva, Vanderlan da S. Bolzani and Ian Castro-Gamboa

Graphical Abstract

A rational and selective method using HPLC-ESI-QToF-MS/MS was developed for the dereplication of phenolic derivatives from *Qualea grandiflora* and *Qualea cordata*. The dereplicated metabolites were selected by previous *in vitro* DPPH assay. Seven flavanones and one benzophenone derivative were detected

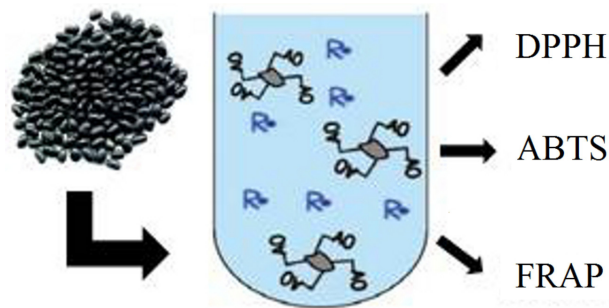


765 Antioxidant Activity of Brazilian Bean Cultivars

Sylvio V. Palombini, Swami A. Maruyama, Thiago Claus, Paula F. Montanher, Nilson E. de Souza, Jesuí V. Visentainer, Sandra Terezinha Marques Gomes and Makoto Matsushita

Graphical Abstract

Legumes of Brazilian origin remain underexplored from the chemical point of view. Thus, this work was aimed at the antioxidant capacity determination of bean cultivars planted in different Brazilian regions through the employment of assays paired with the Quencher procedure. Their fatty acids were also quantified

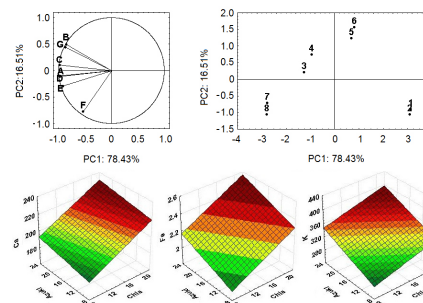


771 Chemometric Methods Applied to the Mineral Content Increase in Chocolate Cakes Containing Chia and Azuki

Aline K. Gohara, Aloisio H. P. Souza, Ângela C. Rodrigues, Gisely L. Stroher, Sandra T. M. Gomes, Nilson E. Souza, Jesuí V. Visentainer and Makoto Matsushita

Graphical Abstract

Experimental design and principal component analysis (PCA) are important chemometric tools that were used to study the increase in mineral contents in cakes due to the use of azuki and chia flours. The response surface and PCA graphs are very useful in facilitating the visualization of the optimal region



777 Multi-Element Analysis, Bioavailability and Fractionation of Herbal Tea Products

Anna Szymczycha-Madeja, Maja Welna and Wieslaw Zyrnicki

Graphical Abstract

The characteristic of macro (C, H, N, S, Ca, Mg, P) and micro (Al, Ba, Cd, Cr, Cu, Fe, Mn, Ni, Pb, Sr, Ti, V) elements and investigations of organic matter in some herbal tea products (including infusions) using spectroscopic methods as well as bioavailabilities and fractionations of elements in teas were presented



788 Aporphine and Tetrahydroprotoberberine Alkaloids from the Leaves of *Guatteria friesiana* (Annonaceae) and their Cytotoxic Activities

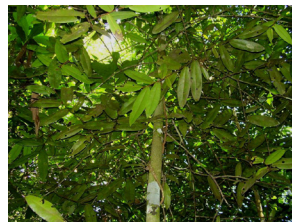


SI online

Emmanuel Vilaça Costa, Pedro Ernesto O. da Cruz, Maria Lúcia B. Pinheiro, Francisco A. Marques, Ana Lúcia T. G. Ruiz, Gabriela M. Marchetti, João Ernesto de Carvalho, Andersson Barison and Beatriz Helena L. N. S. Maia

Graphical Abstract

The phytochemical investigation of the leaves of *Guatteria friesiana* (Annonaceae) afforded three new isoquinoline alkaloids. Eight known alkaloids were also recovered, one of which was isolated as a natural product for the first time. The cytotoxic activity of the extracts, fractions and isolated compounds was evaluated against tumor cell lines

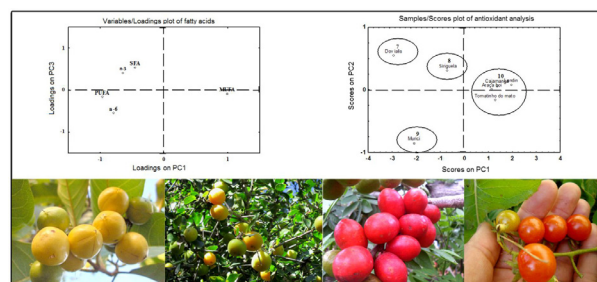


797 Antioxidant Capacity, Total Phenolic Content, Fatty Acids and Correlation by Principal Component Analysis of Exotic and Native Fruits from Brazil

Alessandra B. Ribeiro, Elton G. Bonafé, Beatriz C. Silva, Paula F. Montanher, Oscar O. Santos Júnior, Joana S. Boeing and Jesuí V. Visentainer

Graphical Abstract

Brazil is a country that has favorable geographical and climate characteristics for the production of edible fruits. In this study, the evaluation of exotic and native fruits from Brazil revealed the presence of antioxidant compounds and essential omega-3 and omega-6 fatty acids. Principal component analysis (PCA) helped to differentiate the fruit types

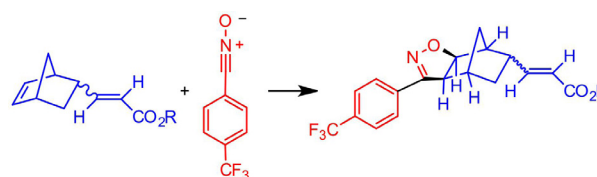


805 NMR Studies on 1,3-Dipolar Cycloaddition of Nitrile Oxides to Norbornenes



SI online

Miroslaw Gućma, W. Marek Gołębiewski and Maria Krawczyk

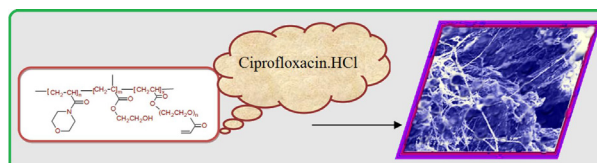


Graphical Abstract

1,3-Dipolar cycloaddition of nitrile oxides to norbornenes substituted with an acrylate moiety occurs with a complete site-selectivity and *exo* selectivity

814 Synthesis of 4-Acryloylmorpholine-based Hydrogels and Investigation of their Drug Release Behaviors

Hülya Efe, Merve Bicen, Memet Vezir Kahraman and Nilhan Kayaman-Apohan



Graphical Abstract

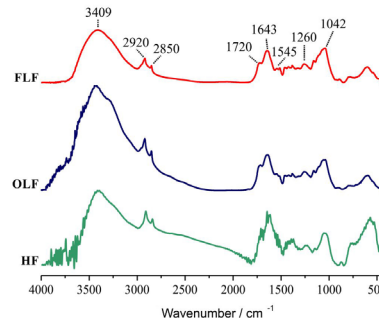
The current study deals with the synthesis of 4-acryloylmorpholine (4-AcM) based hydrogels. Higher drug release was observed by increasing 4-AcM content, whereas the increase in crosslinking density due to PEG-DA content resulted in reduced diffusion of the drug

821 Chemical Composition and Stocks of Soil Organic Matter in a South Brazilian Oxisol under Pasture

Graciele S. Santana, Deborah P. Dick, Michely Tomazi, Cimélio Bayer and Aino V. A. Jacques

Graphical Abstract

Despite the complexity and heterogeneity of the soil organic matter (SOM), spectroscopic and thermogravimetric techniques have been effective tools to give information about its composition and the changes caused by soil use and management



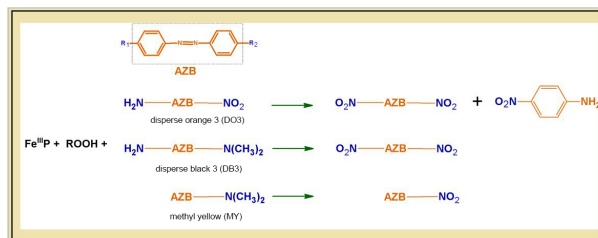
830 Iron Porphyrins as Biomimetical Models for Disperse Azo Dye Oxidation

Valéria P. Barros and Marilda D. Assis

SI online

Graphical Abstract

This paper presents the oxidation of three azo dyes catalyzed by ironporphyrin. The products are resulted from the oxidation of the terminal amine, while the azo bond is left intact and similar products were verified in biological systems

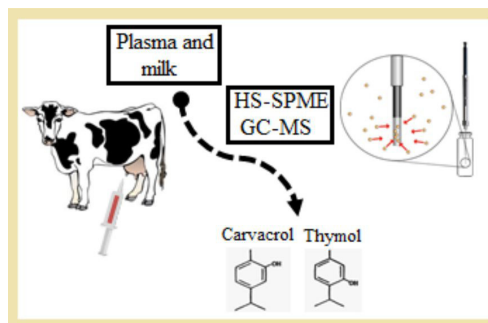


837 Determination of Thymol and Carvacrol in Plasma and Milk of Dairy Cows using Solid-Phase Microextraction

Giovana Maria L. Fiori, Pierina Sueli Bonato, Maria Paula Marques Pereira, Silvia Helena T. Contini and Ana Maria S. Pereira

Graphical Abstract

Development of an analytical method for identification and quantification of thymol and cavacrol in plasma and milk of cows after administration of an intra-mammary phytoformulation of veterinary use containing plant essential oils rich in thymol and cavacrol

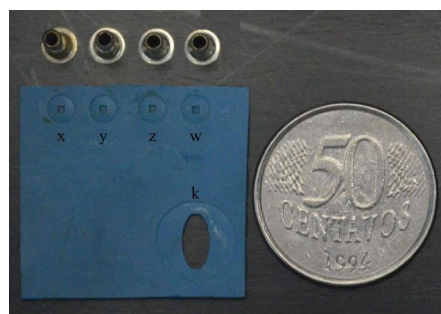


847 A Compact Miniaturized Flow System Based on Low-Temperature Co-fired Ceramic Technology Coupled to LED Mini-photometer for Determination of Dipyrone in Pharmaceutical Formulations

William T. Suarez, Osmundo D. Pessoa-Neto, Vagner B. dos Santos, Ana Rita de A. Nogueira, Ronaldo C. Faria, Orlando Fatibello-Filho and Julián A. Chamorro

Graphical Abstract

Photograph of a typical LTCC (low-temperature co-fired ceramic) device for microfluidic applications. The inlets are indicated by x, y and z, the outlet of the solutions by w and the optical flow cell by k. The cavities for coupling the brass tubes are also shown

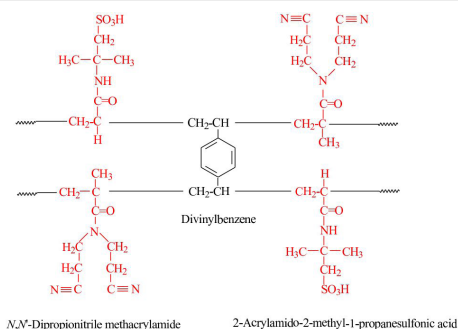


856 Speciation and Preconcentration of Chromium from Water and Food Samples by Synthesized Chelating Resin

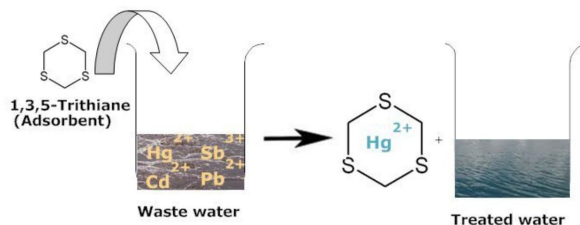
Gökhan Çimen, Şerife Tokaloğlu, İsmail Özentürk and Cengiz Soykan

Graphical Abstract

The preparation of poly(*N,N'*-dipropionitrile methacrylamide-co-divinylbenzene-co-2-acrylamido-2-methyl-1-propanesulfonic acid) resin was carried out with a radical initiator in dimethylformamide solution



- 865 **Removal of Mercury, Antimony, Cadmium and Lead from Aqueous Solution using 1,3,5-Trithiane as an Adsorbent**
Özgen Ercan and Adnan Aydin



Graphical Abstract

1,3,5-Trithiane was used as a new adsorbent for removal of toxic metals such as mercury from wastewater. Adsorption isotherm models were applied to the experimental data

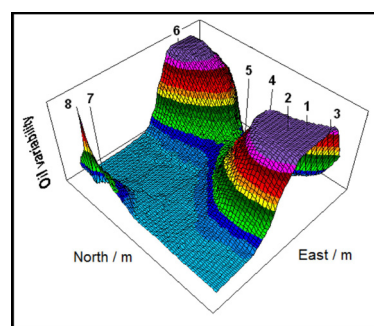
Short Reports

- 873 **Spatial Chemometric Analyses of Essential Oil Variability in *Eugenia dysenterica***

Eliane C. Vilela, Alessandra R. Duarte, Ronaldo V. Naves,
SI online Suzana C. Santos, José C. Seraphin and Pedro H. Ferri

Graphical Abstract

Spatial chemometric methods based on fitted models using variograms and probability maps characterized the spatial chemical structure of *E. dysenterica* essential oil. These methods may contribute as additional tools to establish *in situ* conservation areas or sampling areas for *ex situ* conservation based only on oil chemovariations

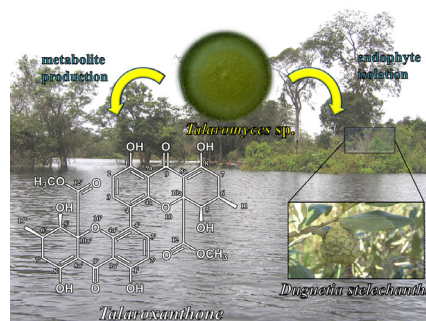


- 880 **Talaroxanthone, a Novel Xanthone Dimer from the Endophytic Fungus *Talaromyces* sp. Associated with *Duguetia stelechantha* (Diels) R. E. Fries**

Hector H. F. Koolen, Laís S. Menezes, Mayane P. Souza,
Felipe M. A. Silva, Fabiana G. O. Almeida, Antonia Q. L. de Souza,
Angelita Nepel, Andersson Barison, Flávio Henrique da Silva,
Danilo Elton Evangelista and Afonso D. L. de Souza

Graphical Abstract

Dimeric xanthones related to the secalonic acids from fungi occur exclusively with C2-C2' connection. On the other hand, phomoxanthones are the only report of dimeric xanthones related to these acids from fungi that have a C4-C4' connection. The novel compound Talaroxanthone (from *Talaromyces* sp.) is the first report of a fungal xanthone dimer from an endophytic fungus with unusual C4-C4' connection and the absence of a methylene group at C12 and C12'



- 884 **Estimation of the Bioaccessibility of Metallic Elements in Chocolate Drink Powder using an *in vitro* Digestion Method and Spectrometric Techniques**

Rafaella R. A. Peixoto, Elaine A. M. Mazon and
Solange Cadore

Graphical Abstract

The *in vitro* simulation of the human digestive process occurring in the mouth, stomach and intestine with the preparation of synthetic digestive fluids containing natural enzymes was studied. This model showed to be a good strategy to assess the bioaccessibility of metallic elements in chocolate drink powder (figure adapted from <http://www.aboutgastro.com/digestive-system>)

