

Cover Picture



Brazilian coffee has reached the level of global high quality coffees, due to scientific studies and advanced agricultural technologies. In this paper, techniques of surface analysis by mass spectrometry (DESI-MS and EASI-MS) in the investigation of green beans Arabica coffees were employed in order to know in detail the constituents of the wax beans, and assess the potential of these techniques in differentiation of post-harvest treatments via multivariate statistics. Details are presented in the Article **Ambient Mass Spectrometry Employed for Direct Analysis of Intact Arabica Coffee Beans** by *Rafael Garrett, Nicolas V. Schwab, Elaine C. Cabral, Brenno V. M. Henrique, Demian R. Ifa, Marcos N. Eberlin and Claudia M. Rezende* on page 1172.

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Editorial

- 1151 **Looking Forward to Improving Gender Equality in Science**
Solange Cadore and Joaquim A. Nóbrega

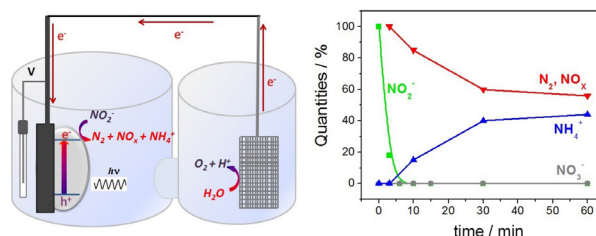
Articles

1153 Efficient Photoelectrochemical Reduction of Nitrite to Ammonium and Nitrogen Containing Gaseous Species Using Ti/TiO₂ Nanotube Electrodes

Fabiana A. Sayão, Luciana Nuñez and Maria V. B. Zanoni

Graphical Abstract

Photoelectrocatalytic reduction of nitrite reached 100% and its conversion involves formation of ammonium ion and nitrogen containing gaseous species by using a two compartment reactor and absence of dissolved oxygen. The procedure is based on UV irradiation of Ti/TiO₂ semiconductor biased with more negative potential than their flat band potential

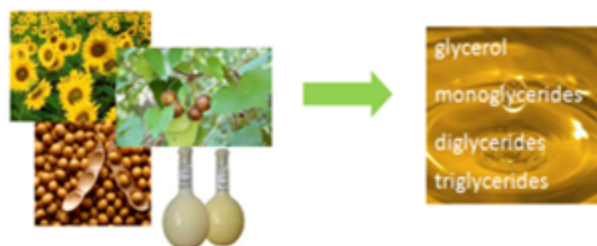


1161 Evaluation of ASTM D6584 Method for Biodiesel Ethyl Esters from Sunflower Oil and Soybean/Tallow Mixture and for Biodiesel Methyl Esters from Tung Oil and Soybean/Tung Mixture

Adriana Neves Dias, Márcia Helena Scherer Kurz, Cássia Alessandra Maciel Fagundes, Sergiane Souza Caldas, Rosilene Maria Clementin, Marcelo Gonçalves Montes D'Oca and Ednei Gilberto Primel

Graphical Abstract

Glycerol and glycerides were determined in samples of biodiesel ethyl esters from soybean/tallow mixture and sunflower and biodiesel methyl esters from soybean/tung mixture and tung oil by employing ASTM D6584 method

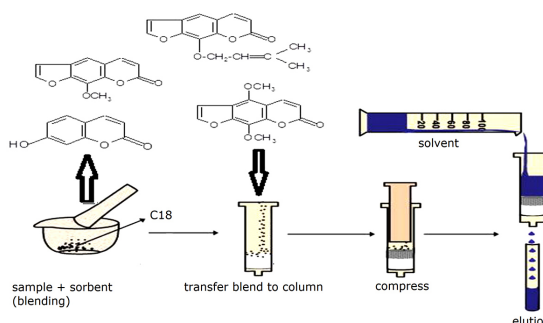


1166 Matrix Solid-Phase Dispersion versus Ultrasound Assisted Extraction with Solid-Phase Extraction in the HPLC Analysis of Furanocoumarins from Fruits of *Archangelica officinalis* Hoffm.

Anna Oniszczuk, Krystyna Skalicka-Woźniak, Tomasz Oniszczuk, Monika Waksmundzka-Hajnos and Kaziemirz Głowniak

Graphical Abstract

A schematic representation of the matrix solid-phase dispersion (MSPD) of furanocoumarins

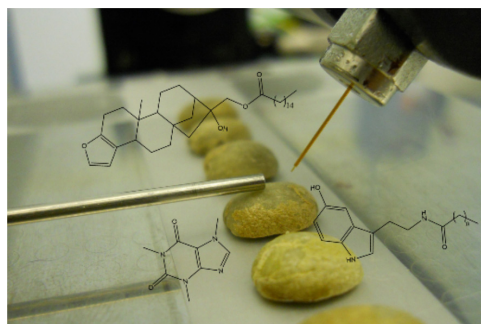


1172 Ambient Mass Spectrometry Employed for Direct Analysis of Intact Arabica Coffee Beans

Rafael Garrett, Nicolas V. Schwab, Elaine C. Cabral, Brenno V. M. Henrique, Demian R. Ifa, Marcos N. Eberlin and Claudia M. Rezende

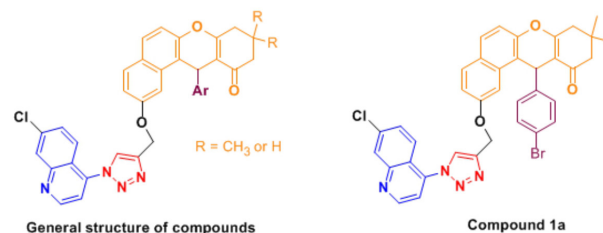
Graphical Abstract

The ambient ionization mass spectrometry techniques DESI and EASI were employed to directly analyze intact beans of Arabica coffees processed by the dry, semi-dry and wet post-harvest treatments



1178 Efficient One Pot Synthesis of Xanthene-Triazole-Quinoline/Phenyl Conjugates and Evaluation of their Antimicrobial Activity

Harjinder Singh, Bhaskara Nand, Jayant Sindhu, Jitender M. Khurana, Chetan Sharma and Kamal R. Aneja

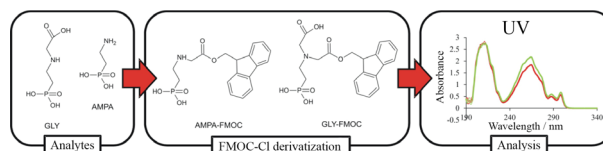


Graphical Abstract

Compound in the right showed best antibacterial and antifungal activity with MIC of 16 $\mu\text{g mL}^{-1}$ against bacteria *Staphylococcus aureus*, *Bacillus subtilis* and also against fungus *Aspergillus niger*

1194 A Simple and Efficient Method for Derivatization of Glyphosate and AMPA Using 9-Fluorenylmethyl Chloroformate and Spectrophotometric Analysis

Tereza C. P. G. Catrinck, Amanda Dias, Maria Clara S. Aguiar, Flaviano O. Silv rio, Paulo H. Fid ncio and Gevany P. Pinho

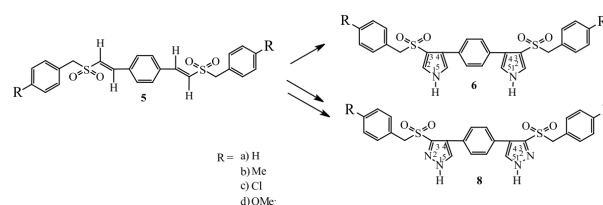


Graphical Abstract

A simple and fast derivatization method for analysis of glyphosate and aminomethylphosphonic acid (AMPA) using UV spectrophotometry

1200 Synthesis and Antioxidant Activity of 1,4-[Bis(3-arylmethanesulfonyl pyrrolyl and pyrazolyl)]benzenes

Gopala Lavanya, Venkatapuram Padmavathi and Adivireddy Padmaja



Graphical Abstract

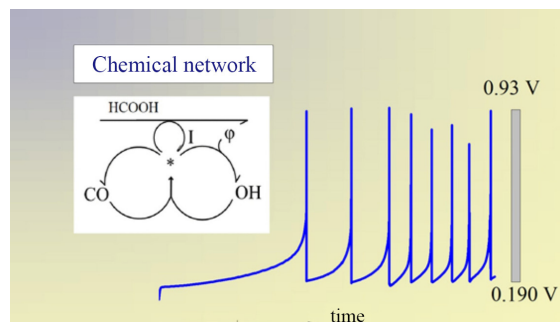
A variety of (1,4-phenylene)bis(arylmethanesulfonylpyrroles and pyrazoles) were prepared by the cycloaddition of 1,3-dipolar reagents, tosylmethyl isocyanide and diazomethane to the Michael acceptor 1,4-bis(E)-2-((arylmethanesulfonyl)vinyl)benzene and evaluated for antioxidant activity. Amongst the tested compounds 5d displayed excellent radical scavenging activity in all the three methods evaluated when compared with the standard ascorbic acid

1208 Complex Electrooxidation of Formic Acid on Palladium

Andressa Mota-Lima, Ernesto R. Gonzalez and Markus Eiswirth

Graphical Abstract

Formic Acid (FA) oscillating mechanism is stressed in the network diagram; competition of CO_{ads} and OH_{ads} by the same free site (*) forms, each one, a loop over the free sites, while direct FA electro-oxidation forms a loop with high turnover rate. Subsurface hydrogen accelerates the direct FA electrooxidation and slows down CO adsorption on Palladium

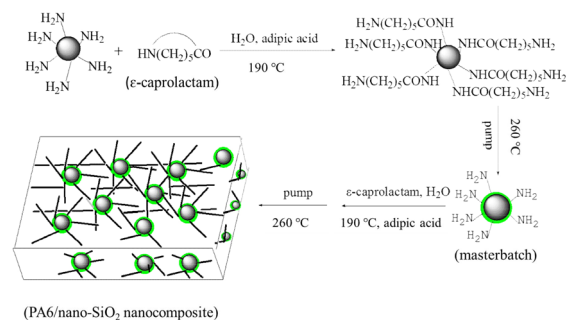


1218 Improving the Mechanical Properties of Polyamide 6-Nanosilica Nanocomposites by Combining Masterbatch Technique with *in situ* Polymerization

Qijie Xu, Xiaohong Li, Fangfei Chen and Zhijun Zhang

Graphical Abstract

A reactive polyamide 6 (PA6)/SiO₂ masterbatch containing 20% (mass fraction) of nano-SiO₂ was used as a filler to prepare polyamide 6/SiO₂ nanocomposites. The as-prepared nanocomposites with 0.5% nano-SiO₂ content presented the best mechanical properties

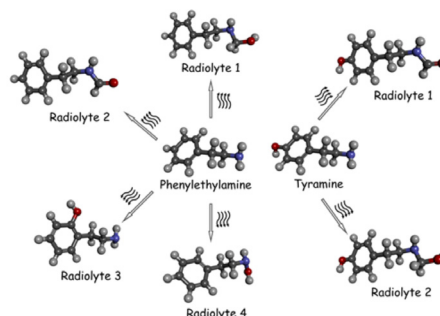


1226 Degradation of Phenylethylamine and Tyramine by Gamma Radiation Process and Docking Studies of its Radiolytes

Monique Cardozo, Stefânia Priscila de Souza, Keila dos Santos Cople Lima, Aline Alves Oliveira, Cláudia Moraes Rezende, Tanos Celmar Costa França and Antonio Luis dos Santos Lima

Graphical Abstract

Degradation products of methanolic and aqueous solutions of phenylethylamine (left) and tyramine (right) by gamma radiation at 5kGy



1237 Antioxidant Capacity in Tilapia Fillets Enriched with Extract of Acerola Fruit Residue

Fabiana Carbonera, Paula F. Montanher, Sylvio V. Palombini, Swami A. Maruyama, Thiago Claus, Hevelise M. C. Santos, Sheisa C. Sargi, Makoto Matsushita and Jesuí V. Visentainer

Graphical Abstract

In the present study, the antioxidant capacity, using different methodologies, and the fatty acid composition of tilapia fillets supplemented with extract of acerola fruit residue were evaluated



1246 A New Spectrophotometric Method for Determining the Enzymatic Activity of endo-β-mannanase in Seeds

Gevany P. Pinho, Juliana R. M. Matoso, Flaviano O. Silvério, Welha C. Mota, Paulo Sérgio N. Lopes and Leonardo M. Ribeiro

Graphical Abstract

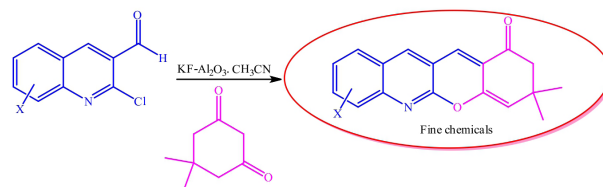
A new spectrophotometric method was developed to determine the enzymatic activity of endo-β-mannanase. A key advantage of the method is that it can be performed with only 5 mg of germinating seeds and hence different parts of the seed can be quickly and efficiently assessed



1253 Efficient Synthesis of Novel Pyranoquinoline Derivatives from Simple Acetanilide Derivatives: Experimental and Theoretical Study of their Physicochemical Properties using DFT Calculations

SI online

Zohreh Mirjafary, Hamid Saidian, Morteza Sahandi and Leila Shojaei



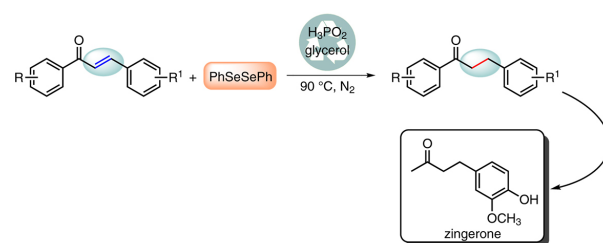
Graphical Abstract

An efficient process for synthesis of pyranoquinolines via Knoevenagel condensation then the ring closures through an addition-elimination reaction of readily available 2-chloroquinoline-3-carbaldehydes with dimedone was reported. On the other hand, NICS values were used as quantitative measures for the relative aromatic character in pyranoquinolines. The results show that NICS for phenyl group of pyranoquinolines are less than that for benzene

1261 Glycerol/Hypophosphorous Acid and PhSeSePh: An Efficient and Selective System for Reactions in the Carbon-Carbon Double Bond of (E)-Chalcones

SI online

Katiúcia D. Mesquita, Bianca Waskow, Ricardo F. Schumacher, Gelson Perin, Raquel G. Jacob and Diego Alves

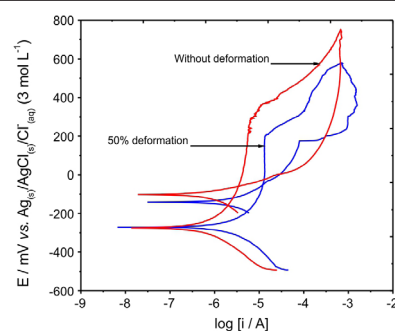


Graphical Abstract

Reaction of *in situ* generated benzeneselenenol with various (E)-chalcones using glycerol as solvent, gave 8-selanylcarbonyl compound or chemoselective 1,4-reduction products, depending on the amount of benzeneselenenol employed and the nature of (E)-chalcone. The glycerol/H₃PO₂ system can be easily recovered and reused in chemoselective 1,4-reductions and the natural product zingerone can be synthesized in good yield

1270 Influence of Cold Deformation on Pitting Corrosion Resistance of ISO NBR 5832-1 Austenitic Stainless Steel Used for Orthopedic Implants

Alexander H. Ramirez, Cristiaann H. Ramirez and Isolda Costa



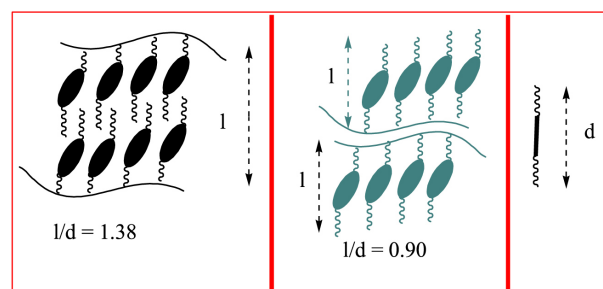
Graphical Abstract

Potentiodynamic polarization curves of the ISO NBR 5832-1 stainless steel with cold deformation (50% reduction in thickness) or without deformation (0%) showing that the cold deformation increased pitting susceptibility of the stainless steel

1275 Side-Chain Liquid-Crystalline Polymer Tetrazoles: Synthesis and Characterization

SI online

Muhammad Tariq, Shahid Hameed, Rachel F. Magnago, Ivan H. Bechtold and Aloir A. Merlo



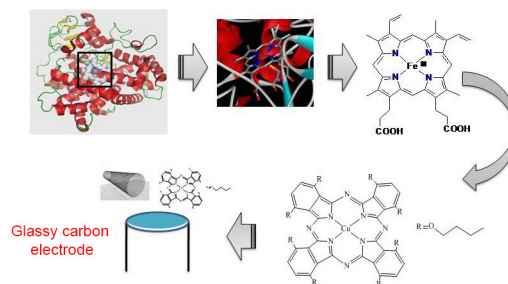
Graphical Abstract

Structure of smectic C (SmC) mesophase determined by X-ray analysis of polymer tetrazoles poly-{4-(2-nonyl-2H-tetrazol-5-yl)phenyl 4-[(propionyloxy)butyloxy]}benzoate (left) and poly-{4-(2-nonyl-2H-tetrazol-5-yl)phenyl 4-[(propionyloxy)undecyloxy]}benzoate (right)

1283 Monitoring of Diclofenac with Biomimetic Sensor in Batch and FIA Systems

Ademar Wong, Luiz D. Marestoni and Maria D. P. T. Sotomayor

SI online



Graphical Abstract

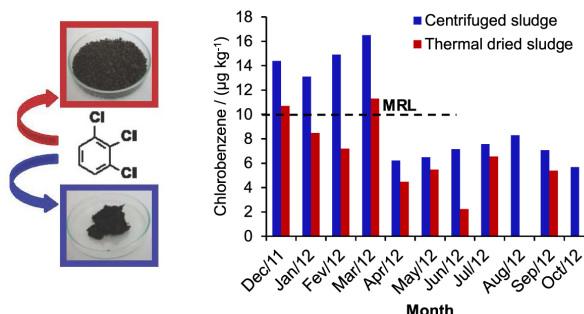
Modification of glassy carbon electrode with MWCNT-COOH and copper phthalocyanine complex, which is responsible for imitating the active site of the P450 enzyme, iron protoporphyrin IX

1292 Determination of Chlorobenzenes in Sewage Sludge by Solid-Liquid Extraction with Purification at Low Temperature and Gas Chromatography Mass Spectrometry

Gevany P. Pinho, Flaviano O. Silvério, Gabriela F. Evangelista, Laila V. Mesquita and Érica S. Barbosa

Graphical Abstract

The technique of solid-liquid extraction with purification at low temperature was used in the monitoring of sewage sludge samples collected within the period of 11 months. The 1,2,3-trichlorobenzene was quantified in concentrations higher than the maximum residue limit for chlorobenzene in soil amended with sludge



1302 The Influence of Salinity and Matrix Effect in the Determination of Antifouling Biocides in Estuarine Waters of Patos Lagoon (Southern Brazil)

Luís A. E. Dominguez, Sergiane S. Caldas, Ednei G. Primel and Gilberto Fillmann

SI online

Graphical Abstract

An analytical method was optimized and applied to analyze the antifouling biocides irgarol and diuron in estuarine and coastal waters under the influence of Rio Grande harbors. The concentrations were lower (< 1.3 to 21 ng L^{-1}) than those capable of causing harm to the aquatic biota

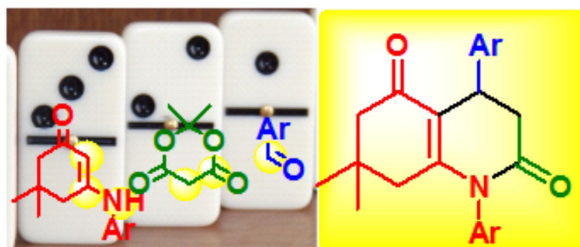


Short Report

1311 Synthesis of Quinolinediones by Catalyst-Free Formal Aza-[3+2+1] Cycloaddition of Enaminones, Aldehydes and Meldrum's Acid

Silvio Cunha and Lourenço L. B. de Santana

SI online



Graphical Abstract

A green procedure to the domino one-pot three-component reaction was developed to the synthesis of 4-aryl-tetrahydroquinoline-2,5-diones