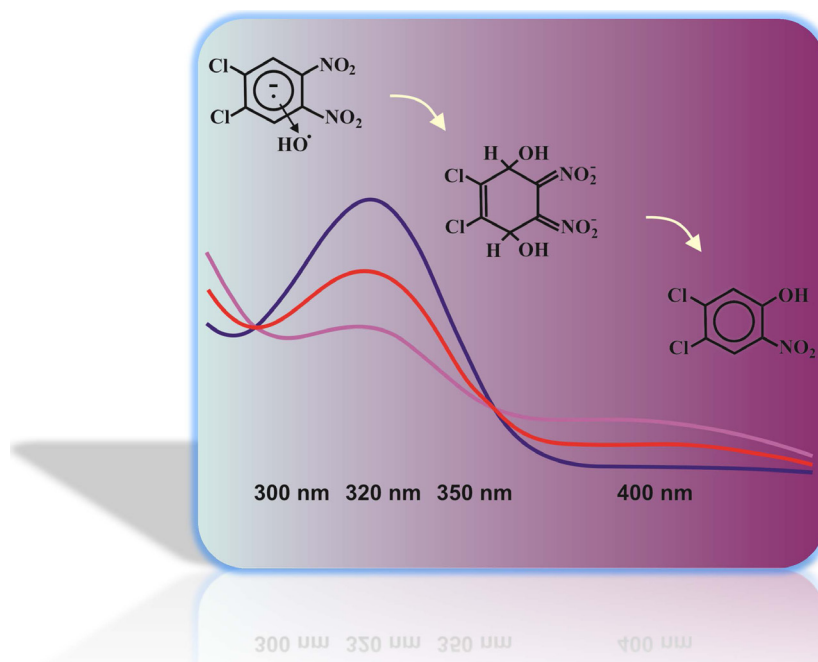


Cover Picture



There is evidence for the Single Electron Transfer Mechanism as an alternative to the classical heterolytic model of aromatic nucleophilic substitution of the reaction of OH^- with 1,2-dichloro-4,5-dinitrobenzene, involving the displacement of nitro group, to form the final product 2-nitro-4,5-dichlorophenol. Details are presented in the Article **The Reaction of 1,2-Dichloro-4,5-dinitrobenzene with Hydroxide Ion: Roles of Meisenheimer Complexes and Radical Pairs** by *Andrei Blaskó, Clifford A. Bunton, Nichollas D. Gillitt, Radu Bacaloglu, Santiago F. Yunes and César Zucco* on page 1146.

Contents

Articles

- 1079** Convenient Solvatochromic Probes for the Determination of Solvent Properties: β -Carotene and 2-Chloro-7-nitro-9H-fluorene

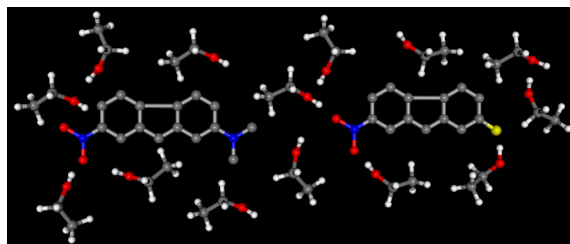
Omar A. El Seoud, Paulo A. R. Pires, Carina Loffredo, Muhammad Imran, Paolo D. Pulcini, Michelle F. Corrêa and Rizwana Mustafa



SI online

Graphical Abstract

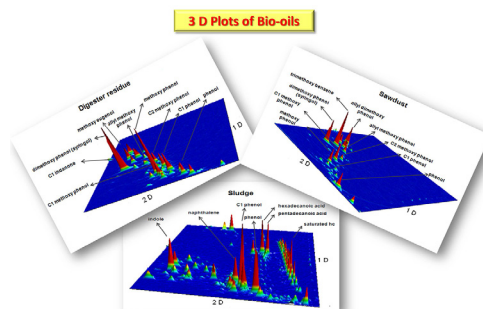
The solvatochromic probes 2-(*N,N*-Dimethylamino)-7-nitro-9H-fluorene and the commercially available β -carotene and 2-chloro-7-nitro-9H-fluorene can be conveniently employed for determining the properties of solvents and their mixtures



- 1085 Comprehensive Two-Dimensional GC with TOF-MS Detection: Study of Pyrolytic Bio-Oil of Kraft Mill Residues**
Candice S. Faccini, Isadora Dalla Vecchia, Desyrre Ribeiro, Claudia A. Zini and Elina B. Caramão

Graphical Abstract

Color plots of bio-oils obtained from pyrolysis of three pulp mill residues and analyzed with comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometric detection (GC×GC/TOFMS) unveil the complexity and potential of these materials for industrial use

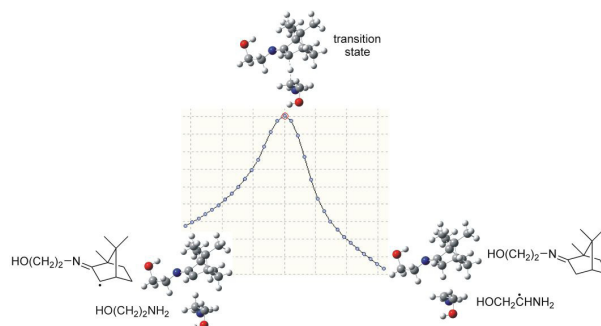


- 1099 Debromination of *endo*-(+)-3-Bromocamphor with Primary Amines**

Svetlana Marković, Violeta Marković, Milan D. Joksović, Nina Todorović, Ljubinka Joksović, Vladimir Divjaković and Snežana Trifunović

Graphical Abstract

Ethanolamine and ethylene diamine debrominate 3-bromocamphor giving the corresponding camphanimines in good isolated yields. The yield of the obtained camphanimines strongly depends on solvent polarity and steric demand of the applied amine. The reaction mechanism was investigated by means of density functional theory (DFT) calculations

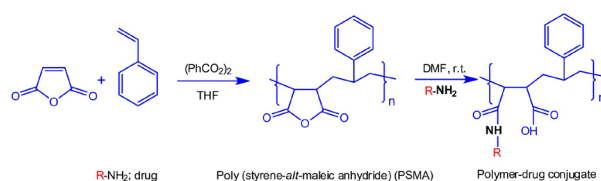


- 1109 Grafting Amino Drugs to Poly(styrene-*alt*-maleic Anhydride) as a Potential Method for Drug Release**

Ardeshir Khazaei, Shahnaz Saednia, Javad Saïen, Masoud Kazem-Rostami, Mahdieh Sadeghpour, Maryam Kiani Borazjani and Fatemeh Abbasi

Graphical Abstract

Novel types of polymer-drug conjugates based on PSMA with pendant medicinal compounds were synthesized, characterized. Hydrolysis reactions were also studied, and then drug release kinetics and mechanisms were reported to introduce a controlled drug delivery system

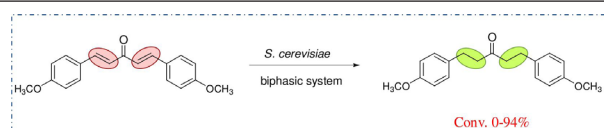


- 1116 Use of *Saccharomyces cerevisiae* Yeasts in the Chemoselective Bioreduction of (1*E*,4*E*)-1,5-Bis(4-Methoxyphenyl)-1,4-Pentadien-3-one in Biphasic System**

César A. Schaefer, Vanessa D. Silva, Boris U. Stambuk and Maria da G. Nascimento

Graphical Abstract

The biotransformation using baker's yeast (BY) from Fleischmann as catalyst in aqueous/organic solvent biphasic system was chemoselective and formed the saturated ketone. The concentration of BY and substrate, temperature, pH and V_{aq}/V_{org} , influenced the reduction, and DMSO was the best co-solvent

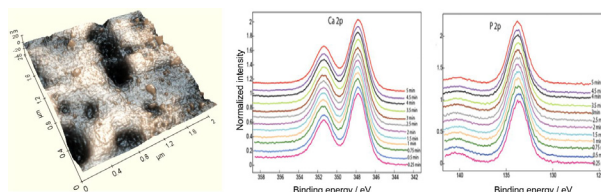


- 1123 Characterization and Corrosion Resistance of Anodic Electrodeposited Titanium Oxide/Phosphate Films on Ti-20Nb-10Zr-5Ta Bioalloy**

Monica Popa, Cora Vasilescu, Silviu I. Drob, Petre Osiceanu, Mihai Anastasescu and Jose M. Calderon-Moreno

Graphical Abstract

AFM micrographs showed that the electrodeposited film has a porous microstructure and good roughness. X-ray photoelectron spectroscopy (XPS) superimposed spectra indicated that the coating deposited over time had a variable composition: nanocrystalline hydroxyapatite nucleated at the inner layer, and amorphous calcium phosphate was formed at the outer layer

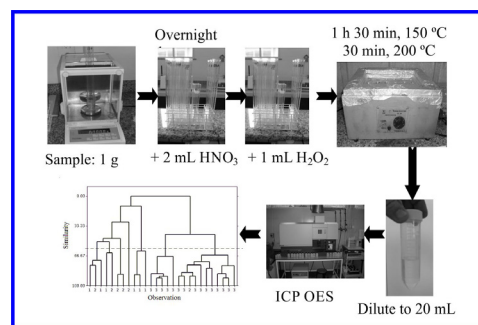


1135 Classification of Honeys from Pará State (Amazon Region, Brazil) Produced by Three Different Species of Bees using Chemometric Methods

Antonio dos S. Silva, Cláudio N. Alves, Kelly das G. Fernandes and Regina C. S. Müller

Graphical Abstract

Flowchart of the analysis of metal contents in samples of honey from bees from Amazonia (Brazil) and dendrogram with separation of the three types of honeys studied

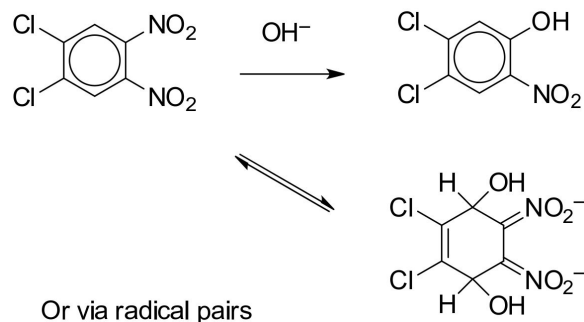


1146 The Reaction of 1,2-Dichloro-4,5-dinitrobenzene with Hydroxide Ion: Roles of Meisenheimer Complexes and Radical Pairs

Andrei Blaskó, Clifford A. Bunton, Nicholas D. Gillitt, Radu Bacaloglu, Santiago F. Yunes and César Zucco

Graphical Abstract

The major reaction of OH^- with 1,2-dichloro-4,5-dinitrobenzene in H_2O -DMSO involves the displacement of the nitro group, and transient Meisenheimer complexes are detected. Free radicals are detected in solvents of low water content, but not under the kinetic conditions

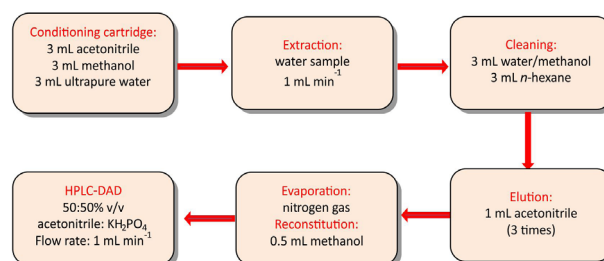


1160 Nonsteroidal Anti-Inflammatory Drug Determination in Water Samples by HPLC-DAD under Isocratic Conditions

Loreto Ascar, Inés Ahumada, Alicia López, Francia Quintanilla and Karla Leiva

Graphical Abstract

The purpose of this study was to implement an analytical method that permits the determination of the presence of nonsteroidal anti-inflammatory drugs (NSAIDs) in water. Compound extraction was performed by solid-phase extraction (SPE) using an Oasis HLB cartridge. Analytes were analyzed by a simple method using HPLC-DAD

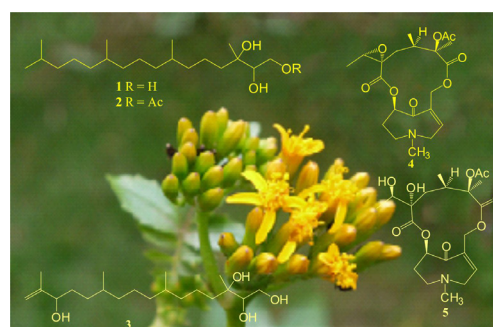


1167 Pyrrolizidine Alkaloids and Diterpenes from *Villasenorina orcuttii*

Amira Arciniegas, Ana L. Pérez-Castorena, Karina González, Marisol Reyes-Lezama, José Luis Villaseñor and Alfonso Romo de Vivar

Graphical Abstract

Two new acyclic diterpenes, as well as the pyrrolizidine alkaloids florosenine and floridanine, among other known compounds, were isolated from *Villasenorina orcuttii*. The absolute stereochemistry of floridanine was determined by X-ray analysis and its NMR data were corrected

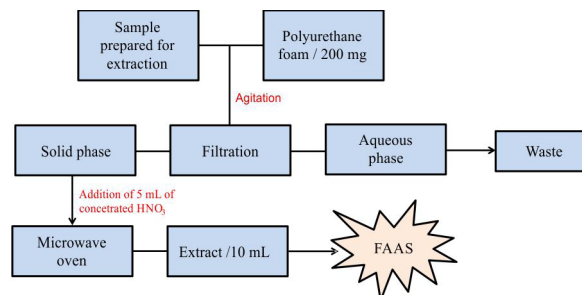


1172 Solid-Phase Extraction of Cu(II) Using Polyurethane Foam and Eriochrome Black T as Ligand for its Determination in Waters by Flame Atomic Absorption Spectrometry

Silvio Soriano and Ricardo J. Cassella

Graphical Abstract

Scheme of the procedure employed for the selective preconcentration of Cu(II) with polyurethane foam and eriochrome black T as ligand, aiming its determination in waters by flame atomic absorption spectrometry

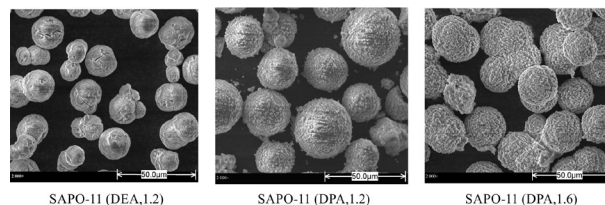


1180 Optimization of the Synthesis of SAPO-11 for the Methylation of Naphthalene with Methanol by Varying Templates and Template Content

Xiaoxiao Wang, Wei Zhang, Shaoqing Guo, Liangfu Zhao and Hongwei Xiang

Graphical Abstract

A set of SAPO-11 zeolites was synthesized by a hydrothermal method using different templates (diethylamine (DEA), di-*n*-propylamine (DPA) and di-isopropylamine (DIPA)) and varying DPA content ($n\text{DPA}/\text{Al}_2\text{O}_3 = 0.8, 1.2, 1.6 \text{ and } 2.0$). SAPO-11(DPA,1.2) exhibited the highest catalytic performance in the methylation of naphthalene with methanol



1188 Multiresidue Determination and Uncertainty Analysis of Pesticides in Soil by Ultrafast Liquid Chromatography Coupled to Mass Spectrometry

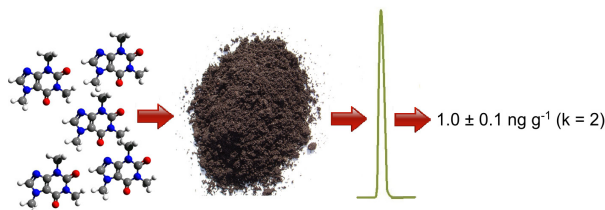


SI online

Diego A. Ahumada, Luis A. Arias and Carlos R. Bojacá

Graphical Abstract

This work shows the results obtained in the validation and characterization of a method for the analysis of pesticide residues in soil by modern analytical techniques. Ultrafast liquid chromatography coupled to mass spectrometry was used, and statistical analysis was performed according to international standards in order to ensure the reliability of the results

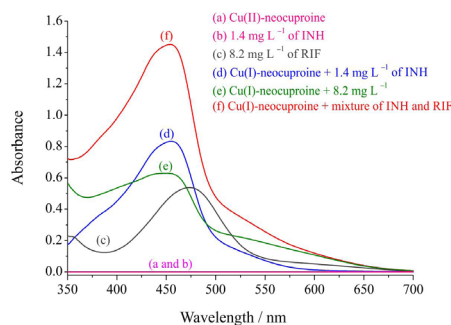


1198 Simultaneous Determination of Rifampicin and Isoniazid in Urine and Pharmaceutical Formulations by Multivariate Visible Spectrophotometry

Sandra Stets, Talita M. Tavares, Patricio G. Peralta-Zamora, Christiana A. Pessoa and Noemi Nagata

Graphical Abstract

A simple chemical derivatization of rifampicin and isoniazid modifies the spectral behavior of these drugs and allows their simultaneous determination using visible spectrophotometry by applying multivariate calibration (PLS)



Short Report

1206 Ultramicroelectrode Array Behavior of Electrochemically Partially Blocked Boron-Doped Diamond Surface



SI online

Giancarlo R. Salazar-Banda, Katlin I. B. Eguiluz, Adriana E. de Carvalho and Luis A. Avaca

Graphical Abstract

Boron-doped diamond electrode surfaces can act as partially blocked or with heterogeneous electroactivity, depending on the polarization, that is, anodic or cathodic, respectively. This was demonstrated using the ferro/ferri-cyanide redox couple at very low scan rates

