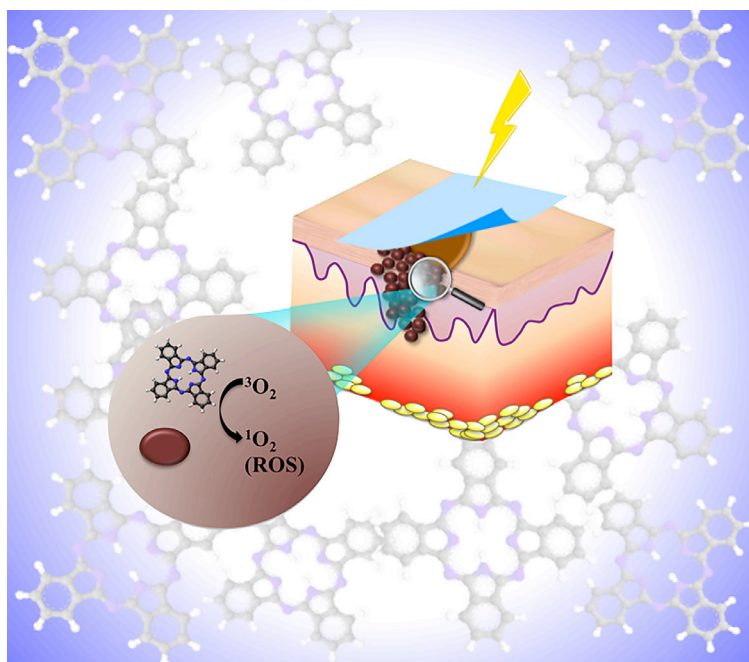


Cover Picture



A drug delivery system based on biocellulose (BC) membranes containing a photosensitizer, chloroaluminum phthalocyanine (ClAlPc), with promising applications in localized topical administration in photodynamic therapy (PDT) is introduced. The non-cytotoxic system is capable to perform the light-induced generation of a reactive oxygen specie (ROS), singlet oxygen ($^1\text{O}_2$), one of the main agents in PDT. Details are presented in the Article **Bacterial Cellulose Membranes as a Potential Drug Delivery System for Photodynamic Therapy of Skin Cancer** by Maristela F. S. Peres, Karina Nigoghossian, Fernando L. Primo, Sybele Saska, Ticiana S. O. Capote, Raquel M. S. Caminaga, Younes Messaddeq, Sidney J. L. Ribeiro and Antonio C. Tedesco on page 1949.

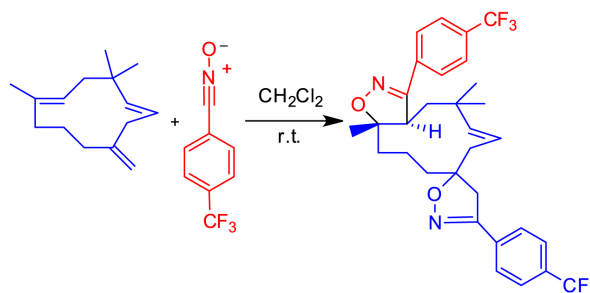
Contents

Articles

1925 NMR Studies on [2 + 3] Cycloaddition of Nitrile Oxides to Polyunsaturated Medium Size Rings

Mirosław Gućma, W. Marek Gołębiewski and Alicja K. Michalczyk

SI online

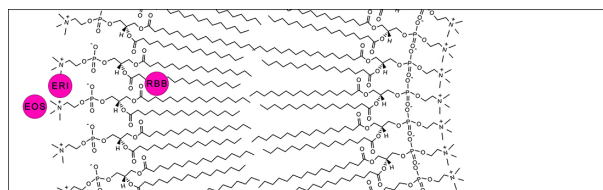


Graphical Abstract

High regio- and site selectivity of [2 + 3] dipolar cycloaddition reaction of 4-trifluoromethylbenzonitrile oxide to C_{15} sesquiterpene was observed.

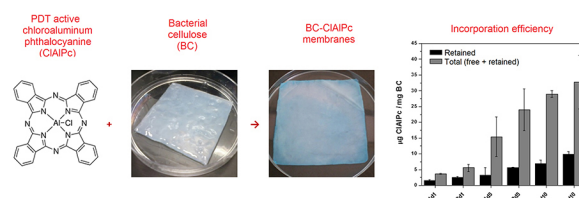
- 1938 Distribution of Xanthene Dyes in DPPC Vesicles: Rationally Accounting for Drug Partitioning Using a Membrane Model**
Italo R. Calori, Diogo S. Pellosi, Douglas Vanzin, Gabriel B. Cesar, Paulo C. S. Pereira, Mario J. Politi, Noboru Hioka and Wilker Caetano

SI online

**Graphical Abstract**

Distribution of xanthene dyes in 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC) vesicles.

- 1949 Bacterial Cellulose Membranes as a Potential Drug Delivery System for Photodynamic Therapy of Skin Cancer**
Maristela F. S. Peres, Karina Nigoghossian, Fernando L. Primo, Sybele Saska, Ticiana S. O. Capote, Raquel M. S. Caminaga, Younes Messaddeq, Sidney J. L. Ribeiro and Antonio C. Tedesco



This drug delivery system has potential for the application in photodynamic therapy (PDT)

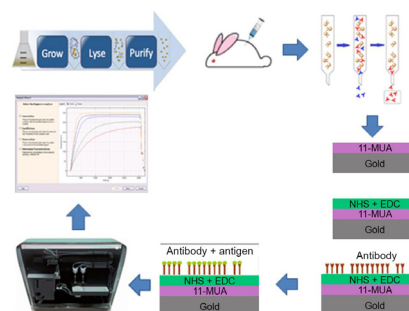
Graphical Abstract

The bacterial cellulose (BC)-chloroaluminum phthalocyanine (CIAIPc) membranes were evaluated as a potential drug delivery system for photodynamic therapy of skin cancer.

- 1960 Development of Surface Plasmon Resonance-Based Immunosensor for Detection of *Brucella melitensis***
Fatemeh Saberi, Mehdi Kamali, Ramezan A. Taheri, Mahdi F. Ramandi, Samira Bagdeli and Reza Mirnejad

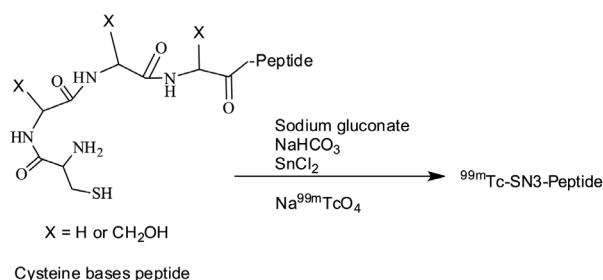
Graphical Abstract

Production and purification of recombinant protein/immunization of rabbit and antibody purification/immobilization of antibody on sensor chip/interaction of bacteria with immobilized antibody/analyzing of responses.



- 1966 Optimizing Labeling Conditions for Cysteine-Based Peptides with ^{99m}Tc**
Hamideh Sabahnou and Seyed Jalal Hosseini-mehr

SI online

**Graphical Abstract**

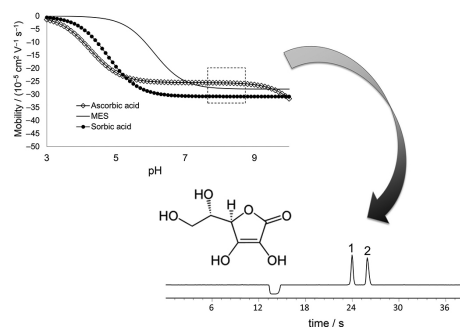
We optimized radiolabeling cysteine-based peptides with technetium- ^{99m}Tc . In this study, the effect of experimental parameters in the labeling procedure such as type of buffer solutions, pH of media, and type of exchange ligands were optimized toward obtaining maximum labeling yield.

1974 A Systematic Procedure to Develop a Capillary Electrophoresis Method Using a Minimal Experimental Data

Daniel A. Spudeit, Samantha Gonçalves, Lizandra C. Bretanha, Carlos A. Claumann, Ricardo A. F. Machado and Gustavo A. Micke

Graphical Abstract

The use of a curve of mobility vs. pH to optimize the optimum background electrolyte (BGE) composition that leads to a reduced analysis time.

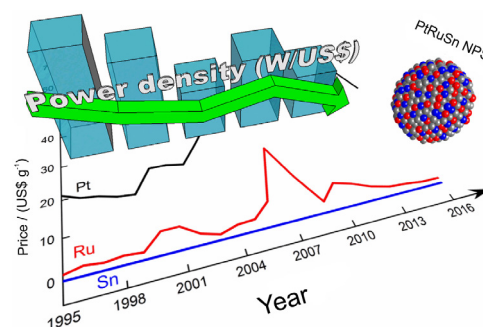


1980 Estimating the Time-Dependent Performance of Nanocatalysts in Fuel Cells Based on a Cost-Normalization Approach

Cinthia R. Zanata, Pablo S. Fernández, Alexandre B. Santos, Gabriel C. da Silva, Giuseppe A. Camara and Cauê A. Martins

Graphical Abstract

A new method to normalize power of fuel cells based on the cost of metals. This method allows the forecasting of power density.

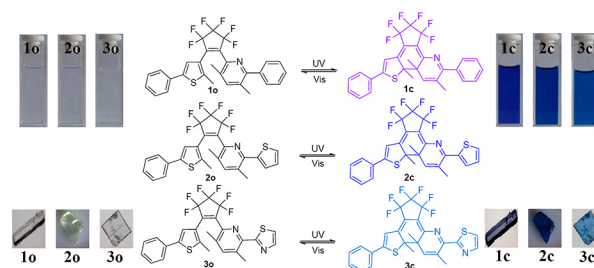


1989 Effects of the Peripheral Heteroaryl Substituents on the Photochromism of New Pyridine-Containing Diarylethenes

Guanming Liao, Dandan Xue, Chunhong Zheng, Renjie Wang and Shouzhi Pu

Graphical Abstract

Three new unsymmetrical diarylethenes were synthesized, exhibiting a notable photochromism. Diarylethenes with thienyl/thiazyl unit showed higher photocyclization quantum yield than that with phenyl moiety, which was ascribed to the existing weak N...S heteroatom-contact.

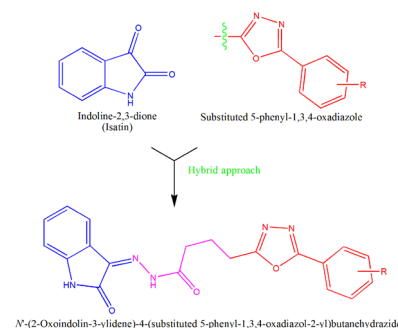


1998 Design, Synthesis, Pharmacological Evaluation and Molecular Docking Studies of Substituted Oxadiazolyl-2-Oxoindolinylidene Propane Hydrazide Derivatives

Deweshri Kerzare, Rupesh Chikhale, Ratnadeep Bansode, Nikhil Amnerkar, Nazira Karodia, Anant Paradkar and Pramod Khedekar

Graphical Abstract

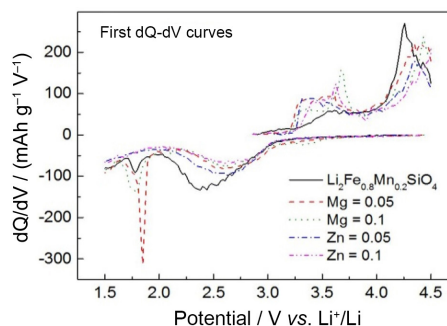
A series of oxadiazolyl-2-oxoindolinylidene propane hydrazides were synthesized based on hybrid approach. Two compounds from this series exhibited good analgesic and anti-inflammatory activity with better protection compared to indomethacin. These compounds also exhibited good dock score of about -4.44 by the K-nearest neighbors (KNN)-genetic algorithm method.



- 2011** **Electrochemical Investigations of $\text{Li}_2\text{Fe}_{0.8-x}\text{Mn}_{0.2}\text{M}_x\text{SiO}_4$ ($\text{M} = \text{Mg}^{2+}, \text{Zn}^{2+}$) Cathodes for Lithium Ion Batteries**
 Shu-Dan Li, Yun Zhao, Chen-Yi Wang and Kun Gao

Graphical Abstract

After the co-doping result in the increasing area of oxidation peak around 3.5 V. At the same time, a shift of reduction peak at 2.5 V towards the right means less internal polarization.



- 2021** **Method Development and Total Uncertainty Estimation for Boron, Sulfur and Phosphorus Determination in Mineral Fertilizer Using ICP OES**

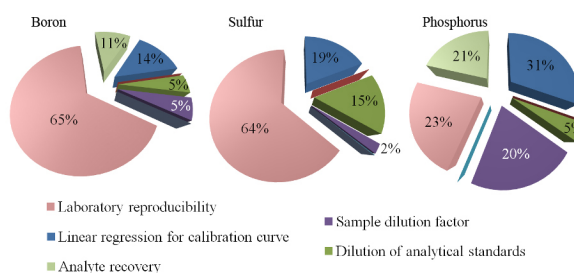


SI online

Tiago C. de Oliveira, Roger T. Rampazzo, Marco F. Ferrão and Dirce Pozebon

Graphical Abstract

Relative contribution of each factor to the total uncertainty in the determination of boron, phosphorus and sulfur in mineral fertilizer by inductively coupled plasma optical emission spectrometry.



- 2034** **Integrated Synthesis of Zeolites Using Coal Fly Ash: Element Distribution in the Products, Washing Waters and Effluent**

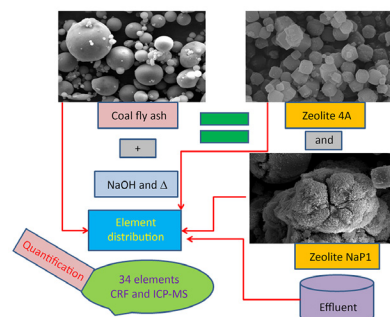


SI online

Suzana F. Ferrarini, Ariela M. Cardoso, Alexandre Paprocki and Marçal Pires

Graphical Abstract

The mobilization of several elements of coal fly ash to end products, washing waters and the effluent of the zeolite two-steps synthesis, was evaluated. The presence of highly toxic elements (As, Cd, Cr, Ni and Pb) in the end products indicates the need for pre-treatment of the ash to ensure a safe zeolite application.



- 2046** **Selective Synthesis of (Z)-Chalcogenoenynes and (Z,Z)-1,4-bis-Chalcogenbuta-1,3-dienes Using PEG-400**

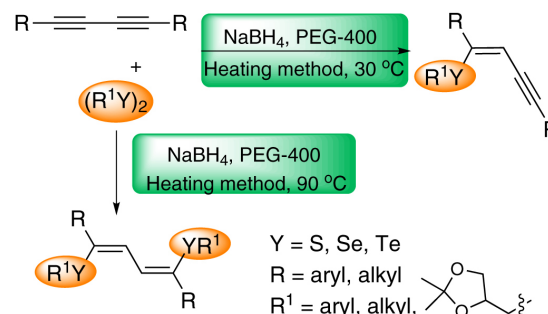


SI online

Renata G. Lara, Liane K. Soares, Raquel G. Jacob, Ricardo F. Schumacher and Gelson Perin

Graphical Abstract

The selective synthesis of (Z)-chalcogenoenynes and (Z,Z)-1,4-bis-chalcogenbuta-1,3-dienes is presented here.

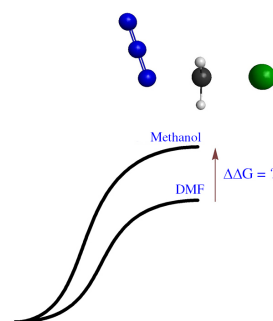


2055 How Accurate is the SMD Model for Predicting Free Energy Barriers for Nucleophilic Substitution Reactions in Polar Protic and Dipolar Aprotic Solvents?

Elizabeth L. M. Miguel, Calink I. L. Santos, Carlos M. Silva and Josefredo R. Pliego Jr.

Graphical Abstract

The solvent model density (SMD) model is not able to predict the protic to dipolar aprotic solvent rate acceleration effect for ion-molecule nucleophilic substitution reactions.

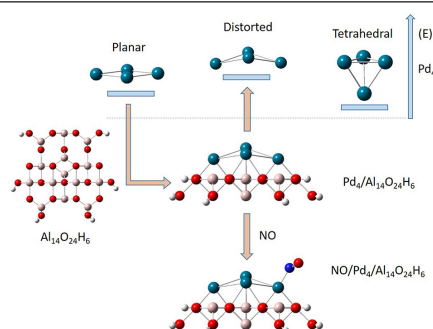


2062 The Effect of Gamma-Al₂O₃ Support on the NO Adsorption on Pd₄ Cluster

Letícia M. Prates, Glaucio B. Ferreira, José W. M. Carneiro, Wagner B. de Almeida, Alexandre N. M. Carauta, Julio C. G. Correia and Maurício T. M. Cruz

Graphical Abstract

Distortion of Pd₄ promoted by γ -alumina cluster (top) and preferential site for adsorption of NO on Pd₄/Al₁₄O₂₄H₆ (bottom).



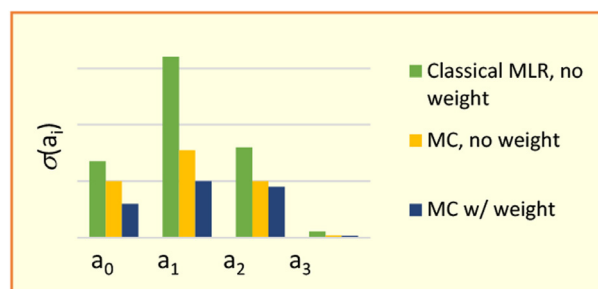
2070 Fighting Collinearity in QSPR Equations for Solution Kinetics with the Monte Carlo Method and Total Weighting

Ruben A. Elvas-Leitão

SI online

Graphical Abstract

Comparison between computed confidence intervals for $\ln k = f(x_1, x_2, x_3)$ regression coefficients.

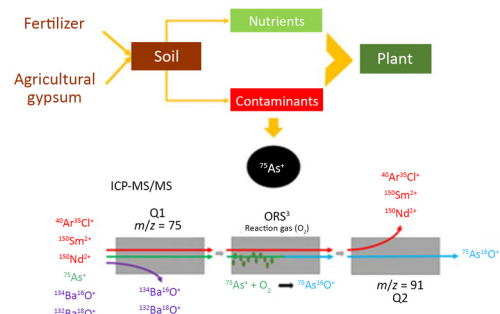


2076 Evaluation of Inductively Coupled Plasma Tandem Mass Spectrometry for Determination of As in Agricultural Inputs with High REE Contents

Raquel C. Machado, Alex Virgilio, Clarice D. B. Amaral, Daniela Schiavo, Joaquim A. Nóbrega and Ana Rita A. Nogueira

Graphical Abstract

Inductively coupled plasma-tandem mass spectrometry (ICP-MS/MS) as an effective tool to overcome double charged interferences from rare earth elements (REEs) on As determination in agricultural inputs.

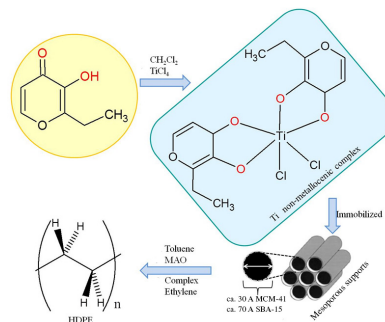


2082 A New Post-Metallocene-Ti Catalyst with Maltolate Bidentate Ligand: an Investigation in Heterogeneous Polymerization Reactions in Different Mesoporous Supports

Grasiela Gheno, Nara Regina de Souza Basso, Paolo Roberto Livotto, Maria Rosário Ribeiro, João Paulo Lourenço, Ana Elisa Ferreira and Griselda Barrera Galland

Graphical Abstract

A new post-metallocene-Ti catalyst with ethylmaltol ligand was synthesized and characterized. This complex was immobilized on different mesoporous supports and investigated in ethylene polymerization reaction giving high density polyethylene.



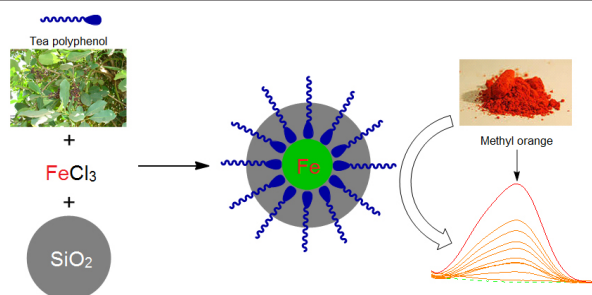
2093 Yerba Mate Tea Extract: a Green Approach for the Synthesis of Silica Supported Iron Nanoparticles for Dye Degradation

Natália S. F. Trotte, Mariana T. G. Aben-Athar and Nakédia M. F. Carvalho

SI online

Graphical Abstract

Iron nanoparticles were prepared from yerba mate tea extract by a green synthetic approach and successfully applied in the degradation of the dye methyl orange.



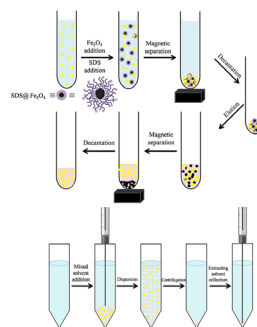
2105 Mixed-Hemimicelle Solid Phase Extraction Followed by Dispersive Liquid-Liquid Microextraction of Amphetamines from Biological Samples

Faezeh Khalilian and Mohammad Rezaee

SI online

Graphical Abstract

A mixed-hemimicelles (MHSPE) method coupled with dispersive liquid-liquid microextraction (DLLME) for the isolation and determination of amphetamines from biological samples is developed based on the use of sodium dodecyl sulfate (SDS)-coated Fe_3O_4 nanoparticles prior to the high performance liquid chromatography (HPLC-UV) analysis.

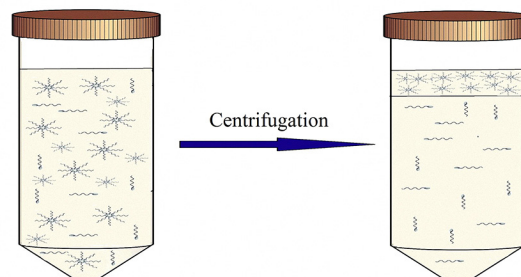


2114 Decanoic Acid Reverse Micelle-Based Coacervates for Microextraction of Silver in Natural Waters Prior to Flame Atomic Absorption Spectrometry Determination

Marzieh Shokouhifar, Seyed Mohammad Hosseini, Mohammad Reza Jamali and Reyhaneh Rahnama

Graphical Abstract

Coacervates made up of reverse micelles of decanoic acid were proposed for the extraction of silver from natural water samples prior to its determination by flame atomic absorption spectrometry (FAAS).

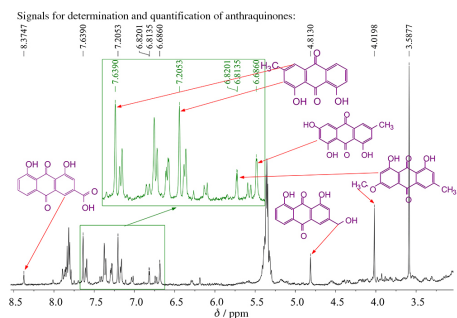


2120 Simultaneous, Simple and Rapid Determination of Five Bioactive Free Anthraquinones in Radix et Rhizoma Rhei by Quantitative ^1H NMR

SI online Jian-Wei Dong, Le Cai, Yun-Shan Fang, Wei-He Duan, Zhen-Jie Li and Zhong-Tao Ding

Graphical Abstract

Five anthraquinones in Radix et Rhizoma Rhei could be quantified accurately using featured signals from ^1H nuclear magnetic resonance (NMR), implying that quantitative ^1H NMR represents a feasible alternative to high-performance liquid chromatography (HPLC)-based methods for quantitation of anthraquinones in Radix et Rhizoma Rhei.

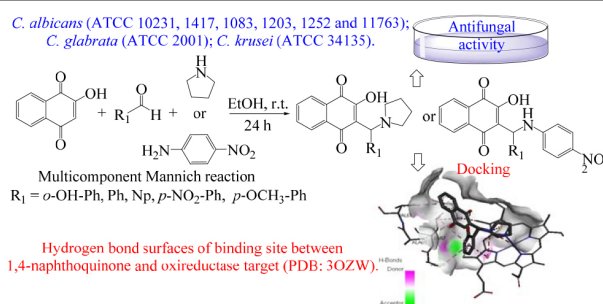


2127 Synthesis, *in vitro* Antifungal Activity and Molecular Modeling Studies of New Mannich Bases Derived from Lawsone

SI online João F. Allochio Filho, Larissa L. Roldi, Maicon Delarmelina, Rodolfo G. Fiorot, Jessica T. Andrade, Alan A. Aleixo, Rafaella S. Carvalho, Marcelo G. F. Araújo, Jaqueline M. S. Ferreira, Alex G. Taranto, Wanderson Romão and Sandro J. Greco

Graphical Abstract

In this work, thirteen Mannich bases derived from lawsone were synthesized. Docking studies and evaluation of the antifungal activity were performed.

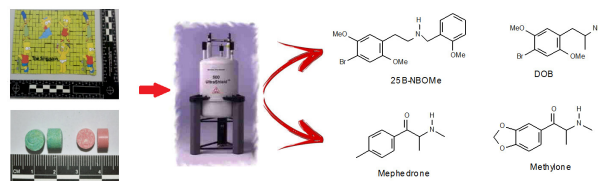


2141 HR-MAS NMR for Rapid Identification of Illicit Substances in Tablets and Blotter Papers Seized by Police Department

SI online Luciano F. Souza, Tarcísio S. Vieira, Glaucia B. Alcantara and Luciano M. Lião

Graphical Abstract

^1H nuclear magnetic resonance (NMR) high-resolution magic angle spinning (HR-MAS) technique represents an important time saver for identification of new synthetic illicit substances seized by police department.



Short Reports

2149 GC×GC-TOF/MS Analysis of Bio-Oils Obtained from Pyrolysis of Acuri and Baru Residues

Claudia Andrea L. Cardoso, Maria Elisabete Machado, Franksteffen S. Maia, Giberto Jose Arruda and Elina B. Caramão

Graphical Abstract

This study is the first report on the analysis of bio-oil from baru and acuri. The samples produced bio-oils with different compositions.

