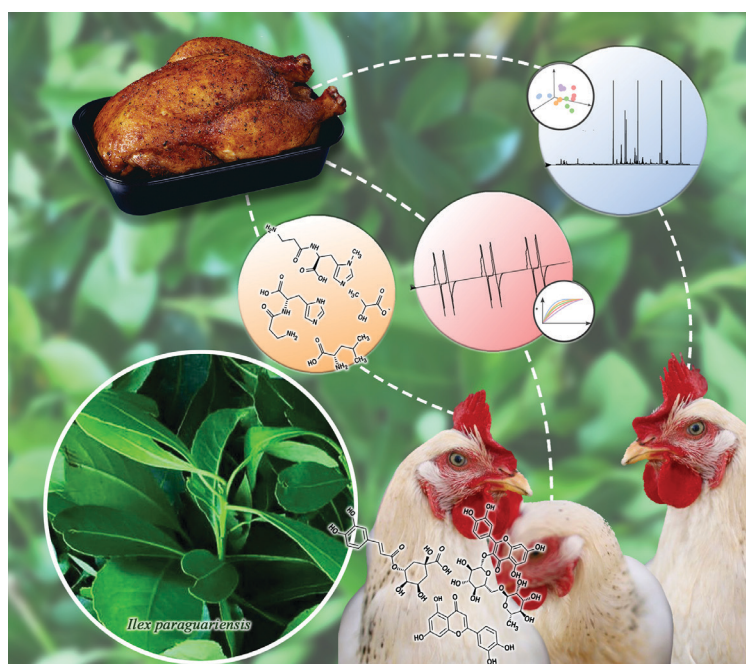


Cover Picture



Mate extract (*Ilex paraguariensis* A.St.-Hil.), generally recognized as safe (GRAS by the FDA), was used as broilers feed additive to improve meat quality and shelf-life. Addition of mate extract to broilers feed affects metabolic pathways related to endogenous peptide derived antioxidants in muscle tissue. Chicken meat from broilers supplemented with lower levels of mate extract (250-500 mg per kg of feed) shows increased content of β -alanine, anserine, and carnosine, improving overall quality and oxidative stability of chicken meat. Details are presented in the Article **Mate as Dietary Supplement for Broiler Chickens: Effect on the Metabolic Profile and Redox Chemistry of Meat** by Caroline Ceribeli, Andressa de Zawadzki, Aline M. C. Racanicci, Luiz A. Colnago, Leif H. Skibsted and Daniel R. Cardoso on page 2266.

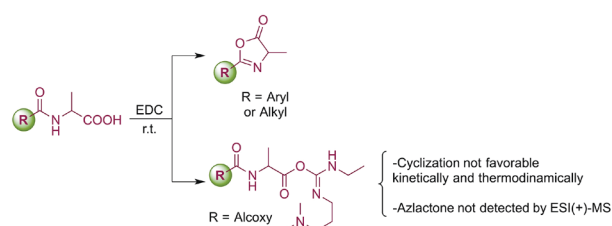
Contents

Communication

2213 Old Drawback on Azlactone Formation Revealed by a Combination of Theoretical and Experimental Studies

Pedro P. de Castro, Gabriel M. F. Batista, Danielle L. J. Pinheiro,
Hélio F. dos Santos and Giovanni W. Amarante

SI online



Graphical Abstract

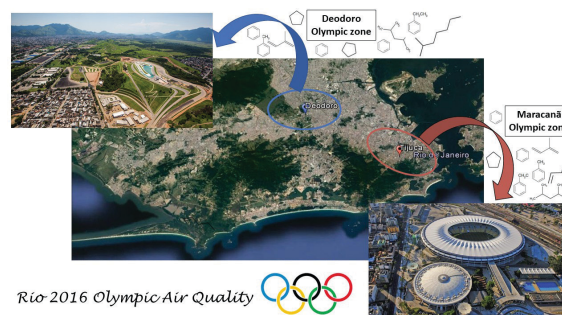
Novel insights in the formation of different 2-substituted azlactone heterocycles. The formation of 2-aryl and 2-alkyl azlactones are favored by a sum of both kinetic and thermodynamic factors, while the cyclization of 2-alkoxy azlactones is less favored.

Articles

2220 Air Quality in the Maracanã and Deodoro Zones During the Rio 2016 Olympic Games

Carolina A. Bezerra, Nicole J. de Carvalho,
Claudio G. P. Geraldino, Cleyton M. da Silva and
Graciela Arbilla

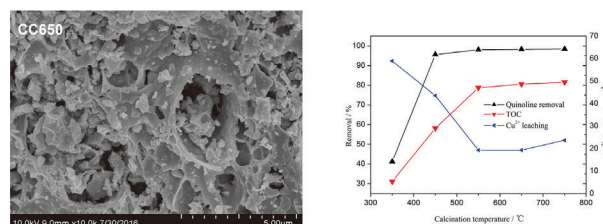
SI online



Graphical Abstract
C₄-C₁₂ non-oxygenated volatile organic compounds and criteria pollutants were analyzed during the Rio de Janeiro Summer 2016 Olympic Games, in two Olympic zones, Maracanã (Tijuca) and Deodoro.

2233 Effect of Calcination Temperature on Catalytic Performance of CeCu Oxide in Removal of Quinoline by Wet Hydrogen Peroxide Oxidation from Water

Zhaojie Jiao, Guilin Zhou, Haidong Zhang, Yu Shen,
Xianming Zhang, Juexuan Li and Xu Gao

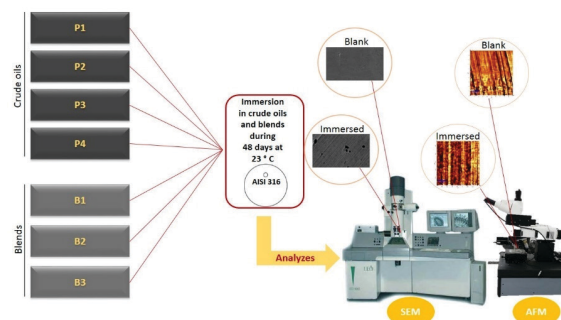


Graphical Abstract
The CeCu-mixed oxide catalyst calcinated at temperature of 650 °C took on the best performance with an oxidation conversion up to 98% for quinoline, a removal efficiency of 80.6% for total organic carbon (TOC) and a low Cu²⁺ leaching value of 19.3 mg L⁻¹.

2244 Study of the Naphthenic Corrosion of AISI 316 and AISI 1020 Steels by Light, Scanning Electron and Atomic Force Microscopies (LM, SEM and AFM)

Débora V. Domingos, Fabrício C. Tozzi, Eliane V. Barros,
Fernanda E. Pinto, Cristina M. S. Sad, Paulo R. Filgueiras,
Valdemar Lacerda Jr., Heloisa P. Dias, Glória M. V. F. Aquije
and Wanderson Romão

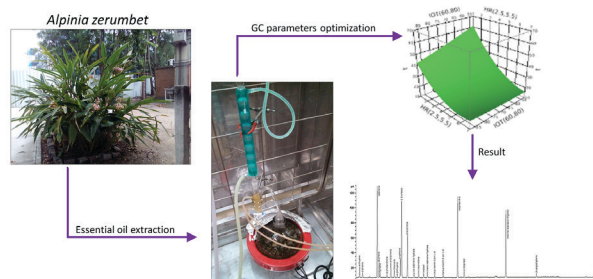
SI online



Graphical Abstract
AISI 316 and AISI 1020 steel coupons were analyzed by scanning electron microscopy (SEM) and atomic force microscopy (AFM) before and after immersion in various crude oil samples and their respective blends for 48 days at room temperature.

2254 Development, Optimization and Validation of a GC Method by Polarity Phase Constants and Statistical Design of Experiments for the Determination of Monoterpenes in *Alpinia zerumbet* Essential Oil

Igor C. Cardoso, Marcos J. Nakamura, Virginia G. Correia,
Henrique M. G. Pereira, Maria D. Behrens and
Marcelo R. R. Tappin

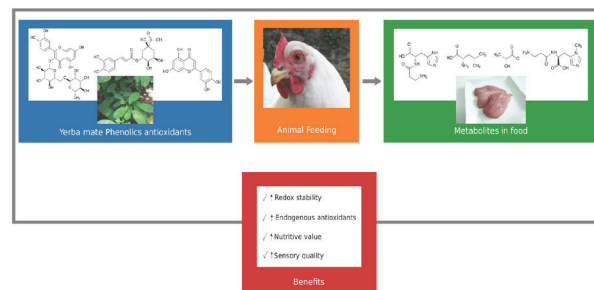


Graphical Abstract
In this report, we described the optimization by response surface methodology of a new analytical method by gas chromatography (GC) for analysis of *Alpinia zerumbet* essential oil.

2266 Mate as Dietary Supplement for Broiler Chickens: Effect on the Metabolic Profile and Redox Chemistry of Meat

Caroline Ceribeli, Andressa de Zawadzki, Aline M. C. Racanicci, Luiz A. Colnago, Leif H. Skibsted and Daniel R. Cardoso

SI online



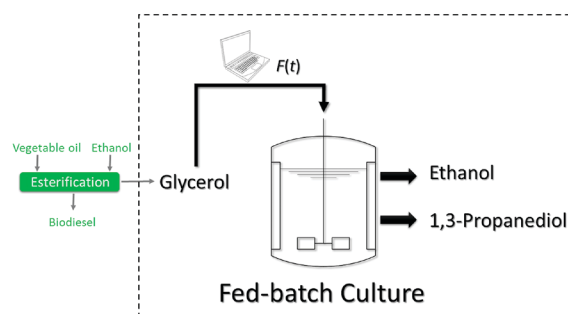
Graphical Abstract

Mate extract in animal diet improves the redox status of meat by changing its metabolic profile towards the production of endogenous antioxidants.

2278 Exponential Fed-Batch Cultures of *Klebsiella pneumoniae* under Anaerobiosis Using Raw Glycerol as a Substrate to Obtain Value-Added Bioproducts

Allan Morcelli, Rosane Rech, Andre Klafke, Rafael Pelegrini and Marco A. Z. Ayub

SI online

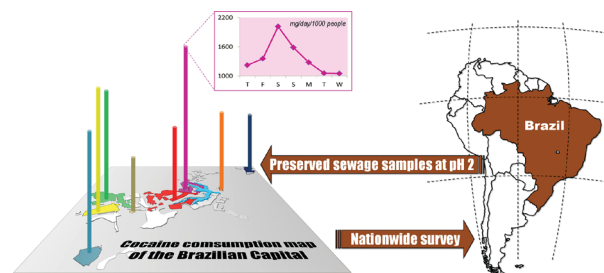


Graphical Abstract

Residual glycerol can be used as substrate in the production of valuable compounds by *Klebsiella pneumoniae* in exponentially fed-batch cultures (EFBC).

2287 Wastewater-Based Epidemiology of Cocaine in the Brazilian Federal District: Spatial Distribution, Weekly Variation and Sample Preservation Strategies

Fernando F. Sodré, Rafael S. Feitosa, Wilson F. Jardim and Adriano O. Maldaner



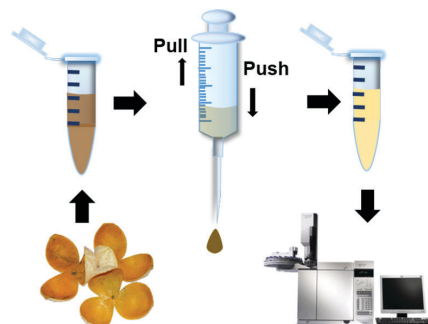
Graphical Abstract

Cocaine use in the Brazilian Federal District, assessed by wastewater-based epidemiology (WBE), revealed higher consumption in the north area, notably during weekends. A nationwide survey may be carried out with sewage samples adjusted to pH 2 and transported within three days under ambient conditions.

2299 Occurrence of Pesticides in Pericarpium Citri Reticulatae and Related Products Using Syringe Filter-Based Cleanup

Fuxin Liu, Xiaowen Dou, Jiaoyang Luo, Dandan Kong, Zhuowen Fan and Meihua Yang

SI online



Graphical Abstract

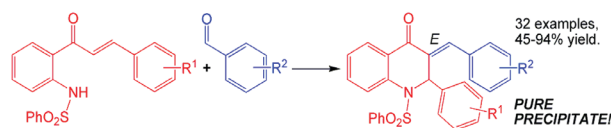
Persistent organochlorines were found in commercial Pericarpium Citri Reticulatae by a “push-and-pull” needle filter based cleanup and gas chromatography (GC) analysis.

2308 **Synthesis, Characterization and Evaluation of *in vitro* Antitumor Activities of Novel Chalcone-Quinolinone Hybrid Compounds**



SI online

Giulio D. C. d'Oliveira, Andrea F. Moura, Manoel O. de Moraes, Caridad N. Perez and Luciano M. Lião

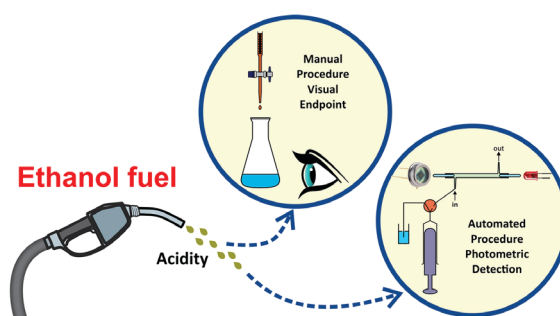


Graphical Abstract

Chalcone-quinolinone synthesis: one step reaction, good yield and pure precipitate.

2326 **Automatic Procedure to Determine Acidity in Fuel Ethanol by Photometric Titration Using Binary Search and Multicommuted Flow Analysis**

Manoel J. A. Lima and Boaventura F. Reis

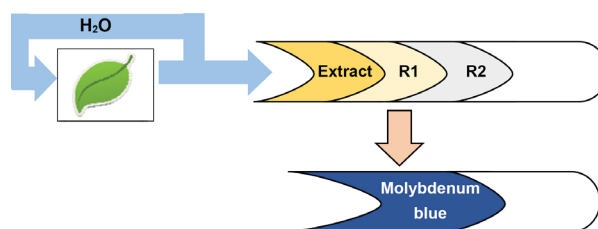


Graphical Abstract

A pictorial overview of the titration procedures for ethanol fuel employing manual and automatic approaches.

2334 **In-Line Incomplete Solid-Liquid Extraction for Spectrophotometric Determination of Soluble Inorganic Phosphorus in Plants and Foods**

Caio C. V. Macedo, Rodrigo S. N. Mancini, Carolina Y. Arakaki and Diogo L. Rocha



Graphical Abstract

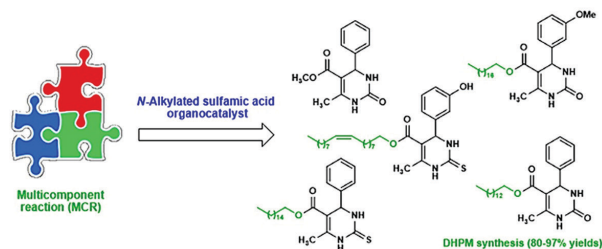
Incomplete and reproducible soluble inorganic phosphorus extraction from vegetable materials and foods prior to spectrochemical analysis in a flow injection analysis (FIA) system with zones penetration.

2342 ***N*-Alkylated Sulfamic Acid Derivatives as Organocatalyst in Multicomponent Synthesis of Fatty Dihydropyrimidinones**



SI online

Carolina R. L. Hack, Larissa Porciuncula, Andressa C. H. Weber, Caroline R. M. D'Oca, Dennis Russowsky, Jaqueline M. Moura, Luiz A. A. Pinto and Marcelo G. M. D'Oca



Graphical Abstract

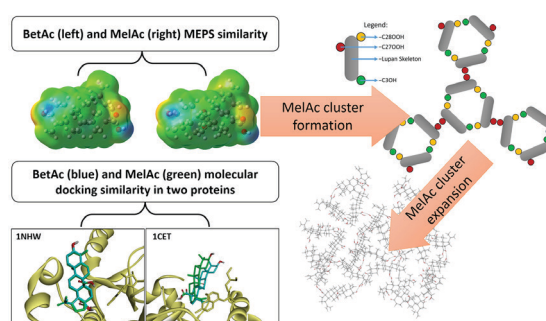
N-Alkylated sulfamic acid derivatives are introduced as promising acidic organocatalysts in multicomponent reactions to the synthesis of dihydropyrimidinones.

2350 Geometry and Stability of Molecular Clusters: Factor to Be Considered in Biomolecular Activity

*Noam G. da Silva, Alexandre M. Alecrim, Renyer A. Costa and
SI online Kelson M. T. de Oliveira*

Graphical Abstract

Molecular clusters are proposed as explanation for the different activities of betulinic and melaleucic acids, compounds with very similar properties.

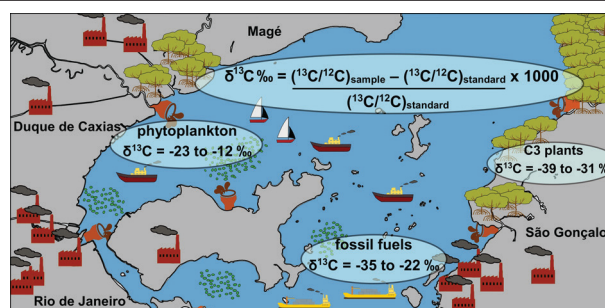


2363 Compound-Specific $\delta^{13}\text{C}$ of *n*-Alkanes: Clean-Up Methods Appraisal and Application to Recent Sediments of a Highly Contaminated Bay

*Milena Ceccopieri, Arthur L. Scofield, Lilian Almeida and
Angela L. R. Wagener*

Graphical Abstract

The image summarizes the $\delta^{13}\text{C}$ equation and the isotopic signature from different carbon sources in the Guanabara Bay, i.e., phytoplankton, mangrove trees, fossil fuel from boat traffic and industries.

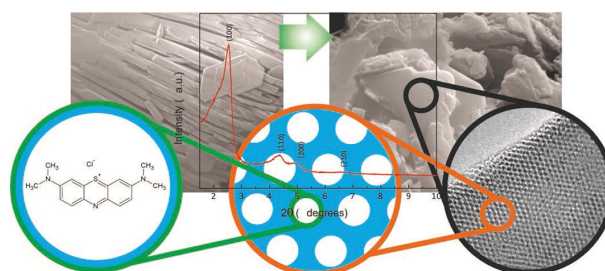


2378 Al-MCM-41 Synthesized from Kaolin via Hydrothermal Route: Structural Characterization and Use as an Efficient Adsorbent of Methylene Blue

*Evânia C. Santos, Luelc S. Costa, Edipo S. Oliveira,
Raquel A. Bessa, Armando D. L. Freitas, Cristiane P. Oliveira,
Ronaldo F. Nascimento and Adonay R. Loiola*

Graphical Abstract

Natural kaolin is efficiently converted, via dealumination and hydrothermal route, to Al-Mobil Composition of Matter No. 41 (Al-MCM-41) mesoporous materials, with a high area surface, showing high performance on methylene blue adsorption from aqueous medium.

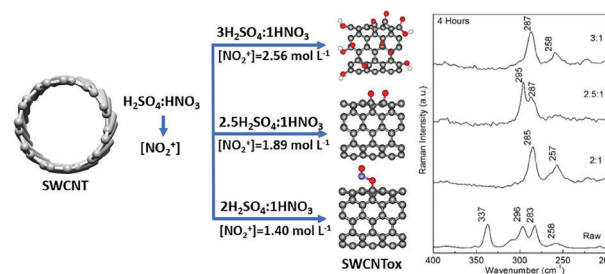


2387 Oxidation of Single-Walled Carbon Nanotubes under Controlled Chemical Conditions

*Arthur B. Porto, Glaucia G. Silva, Hélio F. dos Santos and
Luiz F. C. de Oliveira*

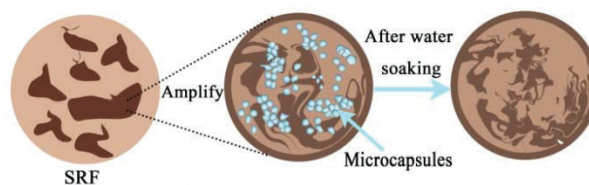
Graphical Abstract

Single-walled carbon nanotubes (SWCNT) are oxidized in acid medium under controlled NO_2^- concentration and reaction time.



2397 Preparation of Microcapsules of Slow-Release NPK**Compound Fertilizer and the Release Characteristics**

Wancheng Pang, Dejia Hou, Huan Wang, Shu Sai,
Baorui Wang, Jingwen Ke, Gaobing Wu, Qing Li and
Mark T. Holtzapple

**Graphical Abstract**

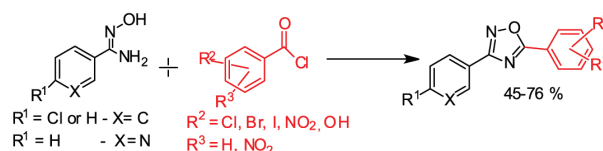
The graphical abstract is an amplified structure of slow-release fertilizer. Microcapsule structure has disappeared after water soaking and the nutrient is slowly released completely.

2405 Synthesis and Antibacterial Evaluation of 3,5-Diaryl-1,2,4-oxadiazole Derivatives

Felipe S. Cunha, Joseli M. R. Nogueira and Alcino P. de Aguiar



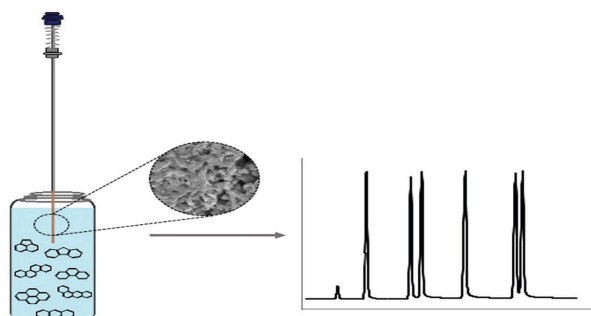
SI online

**Graphical Abstract**

Twenty 1,2,4-oxadiazole derivatives were synthesized and evaluated against five different bacteria.

2417 Use of a Natural Sorbent as Alternative Solid-Phase Microextraction Coating for the Determination of Polycyclic Aromatic Hydrocarbons in Water Samples by Gas Chromatography-Mass Spectrometry

Natália G. Suterio, Sângela N. do Carmo, Dilma Budziak,
Josias Merib and Eduardo Carasek

**Graphical Abstract**

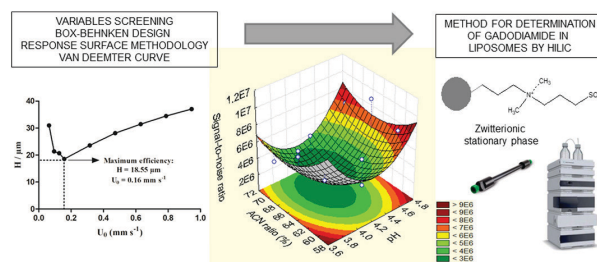
In this study, the use of a biosorbent-based coating in solid-phase microextraction was proposed for the determination of polycyclic aromatic hydrocarbons in water samples.

2426 Chemometric-Assisted Hydrophilic Interaction Chromatographic Method for the Determination of Gadolinium-Based Magnetic Resonance Imaging Contrast Agent in Liposomes

Ana Luíza C. Maia, Pedro Henrique R. da Silva,
Christian Fernandes, Aline T. M. e Silva,
André Luís B. de Barros, Daniel Cristian F. Soares
and Gilson A. Ramaldes



SI online

**Graphical Abstract**

Development, using chemometrics tools, of a hydrophilic interaction chromatographic method for the determination of gadodiamide in liposomes.

2441 Simultaneous Determination of Four Antibiotics in Raw Milk by UPLC-MS/MS Using Protein Precipitation as Sample Preparation: Development, Validation, and Application in Real Samples

Thiago Magon, Roberta da Silveira, Marília B. Galuch,

Eder Paulo Fagan, Ana Flavia D. Feitoza, Sylvio V. Palombini,

Oscar O. Santos and Jesui V. Visentainer

Graphical Abstract

Determination of tetracycline, oxytetracycline, penicillin G and ceftiofur in raw milk by ultra-performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS) using protein precipitation as sample preparation: development, validation, and application in raw milk samples from dairy cows medicated with tetracycline (24, 48, 72 and 96 h after treatment) for subclinical mastitis.

