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## **Cover Picture**



Ecstasy is a term typically used to describe drugs of abuse containing 3,4-methylenedioxymethamphetamine (MDMA). Recently, the trafficking of ecstasy tablets has grown and considerable higher amounts have been seized in Brazil. Herein, we present the development and validation of a <sup>1</sup>H-qNMR (quantitative nuclear magnetic resonance of hydrogen) analytical forensic method capable both to identify and quantify MDMA in ecstasy tablets. Details are presented in the Article **A Validated NMR Approach for MDMA Quantification in Ecstasy Tablets** by *Nathalia S. Almeida, Luiz E. C. Benedito, Adriano O. Maldaner and Aline L. de Oliveira* on page 1944.

## Contents

## **Communication**





Graphical Abstract An efficient and non-expensive method for conversion of diverse potassium organotrifluoroborates to their corresponding boronic acids and boronic esters promoted by montmorillonite K10 using water as the reaction solvent is described.

## Articles

# 1786

In vitro Analysis of the Interaction between Human Serum Albumin and Semi-Synthetic Clerodanes Otávio A. Chaves, Áurea Echevarria, Andressa Esteves-Souza,

Sl online Maria A. M. Maciel and José C. Netto-Ferreira

#### **Graphical Abstract**

The interaction between human serum albumin (HSA) and semi-synthetic clerodanes showing potential anti-cancer activity was evaluated by experimental and theoretical methods. The clerodanes derived from trans-dehydrocrotonin (t-DCTN), methyl-hydrazone (MHDCTN) and phenyl-hydrazone (PHDCTN), showed better binding ability than the natural product *t*-DCTN.



#### **Graphical Abstract**

Selective, simple and fast determination of colchicine by multiple pulse amperometry coupled to flow injection analysis (FIA-MPA) system in pharmaceutical formulations and urine samples using a boron-doped diamond electrode.

1803 Microstructure by Thermal Attack under Vacuum of a Superduplex Stainless Steels and Electrochemical Behavior in H<sub>2</sub>S/CO<sub>2</sub>-Saturated Synthetic Seawater

Elki C. Souza, Carlos A. Fortulan and João M. D. A. Rollo

#### Graphical Abstract

Superduplex stainless steels composed in both equal fraction ferritic-austenite phases are applied as components for use in petrochemical industries in off-shore platforms and its corrosion resistance (due to the passive film on the surface) is dependent on the temperature and environment in which they are exposed.









1811 Palladium Nanoparticles within Core-Cross-Linked Polymer Gels for Suzuki Coupling Reactions: from Monomers to **Ready-to-Use Catalysts in Two-Steps** 

> Tanize Bortolotto, Gabrielly E. Neumann, Suelen G. Trindade, Laura C. E. da Silva, Oscar E. D. Rodrigues, Vanessa Schmidt and Cristiano Giacomelli

#### **Graphical Abstract**

Well-defined cross-linked polymeric structures behaving as highly hydrated unimolecular objects (polymer nanogels) are suitable capping agents for palladium nanoparticle catalyst systems. This structurally complex catalyst composite can be prepared in two-steps.



**3** Solid State Reaction of Serpentinite Mg<sub>3</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub> with NaOH to Produce a New Basic Catalytic Phase Na<sub>2</sub>Mg<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> for Biodiesel Production

SI online Gilvan M. Paz, Sara S. Vieira, Alexandre C. Bertoli, Fabiane C. Ballotin, Edmilson M. de Moura, Ana Paula C. Teixeira, Demétrio A. S. Costa, Ottávio Carmignano and Rochel M. Lago



#### **Graphical Abstract**

The nature of the catalytic site is not clear, but one can consider that in the Na<sub>2</sub>Mg<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> structure is forming a species Si-O·Na<sup>+</sup>. One possible mechanism is the interaction of CH<sub>3</sub>OH with the basic site Si-O·Na<sup>+</sup>.

1830 Optimization of Experimental Parameters in Analysis of Pharmaceutical Pellets by Near Infrared-Chemical Imaging (NIR-CI) and Multivariate Curve Resolution with Alternating Least Squares (MCR-ALS) José Augusto Da-Col and Ronei J. Poppi



Graphical Abstract In this study, the evaluation of multivariate curve resolution with alternating least squares (MCR-ALS) parameters was important for the analysis results of pharmaceutical pellets composition.

1842 Supramolecular Characterization of Humic Acids Obtained through the Bacterial Transformation of a Low Rank Coal Nelson O. Valero, Liliana C. Gómez and Luz M. Melgarejo

## Graphical Abstract

The characterization of humic acid (HA) obtained by activity of bacterial strains, that transform a low rank coal (LRC) lignite type and release humified organic matter (HOM), was compared with HA obtained by the traditional alkaline extraction method using 0.5 M NaOH (HA-NaOH).





Sl online Fernando F. Sodré, Joyce S. Santana, Thiago R. Sampaio and Cristina C. S. Brandão

Graphical Abstract

This work shows the distribution of selected micropollutants in Paranoá Lake that receives effluents from the capital of Brazil and will be used to produce drinking water in order to avoid water scarcity. Source and drinking waters were also investigated.





Volatile Profile of Sparkling Wines Produced with the Addition of Mannoproteins or Lees before Second Fermentation Performed with Free and Immobilized Yeasts Gustavo P. Costa, Karine P. Nicolli, Juliane E. Welke, SI online Vitor Manfroi and Claudia A. Zini



**Graphical Abstract** The use of immobilized yeasts and aging on mannoproteins or lees seemed to be a promising treatment to achieve positive aroma notes in the volatile profile of sparkling wines.



Lilian F. M. do Amaral, Rhaísa T. Betim, Maria G. Nascimento and Cristiane Pilissão

#### Graphical Abstract

The systems Burkholderia cepacia lipase (BCL) on pristine or functionalized multi-walled carbon nanotubes (MWCNTs) resulted in a 3-fold improvement in the conversion and in a 5-fold improvement in ee, (enantiomeric excess of the substrate), when compared with free BCL. The support was reused for eight cycles. An increase in the thermal stability of BCL was confirmed by thermogravimetric analysis (TGA).



1885 Application of Factorial Design and Desirability Function to **Develop a Single Analytical Procedure for the Determination** of Metals in Different Tissues of Blue Crab (Callinectes danae) Daniel C. Lima, Wesley N. Guedes, Vinicius C. Costa and Fábio A. C. Amorim

#### **Graphical Abstract**

Graphical abstract shows the three studied tissues, the sequence of scientific work with relation to the investigation on single condition to prepare samples, analytical features, validation of analytical procedure and application.







Nanorods Formation

**Graphical Abstract** The smaller nanoparticles aggregate to form the nanorods by growth via the targeted binding mechanism.

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1927 Improving Antioxidant Activity of *Ophioglossum thermale* Kom. by Fermentation with *Talaromyces purpurogenus* M18-11

Jian-wei Dong, Le Cai, Xue-jiao Li, Rui-feng Mei, Ping Luo and Zhong-tao Ding



Antioxidant

TPC

Flavonoids

Fermented

Graphical Abstract Ophioglossum thermale Kom. was fermented with Talaromyces purpurogenus M18-11. T. purpurogenus is an effective strain to process O. thermale for improving the antioxidant activity.



SI online Luciana T. D. Cappelini, Juliana V. Alberice, Patrícia F. M. Eugênio, Eloisa Pozzi, Ana Carolina Urbaczek, Lia G. R. Diniz, Elma N. V. M. Carrilho, Emanuel Carrilho and Eny M. Vieira

#### **Graphical Abstract**

A QuEChERS/GC-MS method was essential to quantitate the biological degradation of fipronil in soil fertilized with humic substances. We isolated more than two-dozens of microorganisms from such soil, and the most abundant, *Burkholderia thailandensis*, showed the capability to degrade fipronil into active metabolites.



#### J. Braz. Chem. Soc.



Sl online and Aline L. de Oliveira

**Graphical Abstract** An internal standard <sup>1</sup>H-qNMR (quantitative nuclear magnetic resonance) method was developed and validated for simple, accurate and fast quantification of 3,4-methylenedioxymethamphetamine (MDMA) in seized ecstasy tablets.

The Chemical Composition of Winter Fogs at São Paulo

Pérola C. Vasconcellos, Fábio L. T. Goncalves,

Simone G. Avila, Vitor K. Censon and Heidi Bauer

#### **Graphical Abstract**

Fog sampler, an equipment used to collect fog samples at 2 roads in São Paulo City. Collected droplets coalesce and run down the strands, aided by gravity and aerodynamic drag, into a Teflon® sample trough.



1951

**Highway Sites** 

Sub-Minute Method for Determination of Naphazoline in the Presence of Diphenhydramine, Pheniramine or Chlorpheniramine by Capillary Electrophoresis

Sl online Michelle M. A. C. Ribeiro, Mariana C. Marra, Brenda M. C. Costa, Thiago C. Oliveira, Alex D. Batista, Rodrigo A. A. Muñoz and Eduardo M. Richter

#### **Graphical Abstract**

This work presents a simple and low-cost capillary electrophoresis (CE) method for ultra-fast (< 1 min) simultaneous determination of naphazoline in the presence of diphenhydramine or pheniramine or chlorpheniramine.





Alver A. Castillo-Aguirre, Betty A. Velásquez-Silva, Sl online Cindy Palacio, Frank Baez, Zuly J. Rivera-Monroy and Mauricio Maldonado

NaOH DMF No Reaction

**Graphical Abstract** Regioselective modification of poly(2,3-epoxypropyl methacrylateco-ethylene glycol dimethacrylate-co-methyl methacrylate) (poly(GMA-co-EDMA-co-MMA)) with resorcarenes.





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#### **Graphical Abstract**

Determination of the total amount of heavy metals present in soils is not a good index to estimate the bioavailability and toxicity of these elements. This work describes the use of the Mehlich-1 extractor for evaluating the availability of Cu, Zn, Mn, Ni, Cr and Cd in soil.

