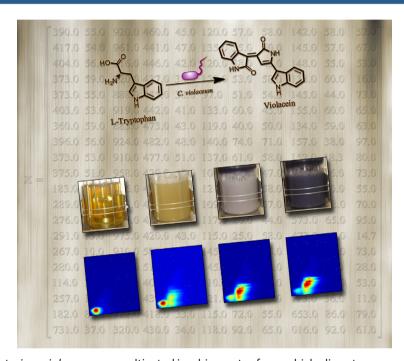
# JBCS

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Journal of the Brazilian Chemical Society Vol. 23, No. 11, November, 2012

# **Cover Picture**



A culture of *Chromobacterium violaceum* was cultivated in a bioreactor from which aliquots were collected every two hours and analyzed by multi-wavelength fluorescence spectroscopy. The mechanistic investigation of the violacein biosynthesis was then performed by the chemometric method parallel factor analysis (PARAFAC) that was applied to resolve the fluorescence profiles. Details are discussed in the Article **The Violacein Biosynthesis Monitored by Multi-Wavelength Fluorescence Spectroscopy and by the PARAFAC Method** by *Clecio Dantas, Pedro L. O. Volpe, Nelson Durán and Márcia M. C. Ferreira* on page 2054.

## **Contents**

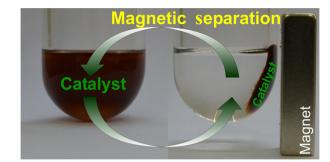
**Editorial** 

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#### Account

1959 Recent Advances in the Development of Magnetically **Recoverable Metal Nanoparticle Catalysts** 

Liane M. Rossi, Marco A. S. Garcia and Lucas L. R. Vono



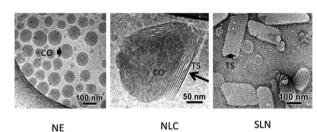
#### **Graphical Abstract**

The immobilization of catalytic active species (metal nanoparticles, metal complexes, enzymes, organocatalysts, etc.) on superparamagnetic nanoparticles allows the facile separation of catalysts from the reaction mixture with the application of an external magnetic field

#### **Articles**

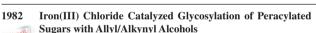
Physicochemical and Morphological Characterizations of Glyceryl Tristearate/Castor Oil Nanocarriers Prepared by the Solvent Diffusion Method

> Cristiana L. Dora, Jean-Luc Putaux, Isabelle Pignot-Paintrand, Frédéric Dubreuil, Valdir Soldi, Redouane Borsali and Elenara Lemos-Senna



#### **Graphical Abstract**

Structural characterizations of drug lipid nanocarriers made from castor oil (CO) and tristearin (TS). NE: nanoemulsions, NLC: nanostructured lipid carriers, SLN: solid nanocarriers





Senthil Narayanaperumal, Rodrigo César da Silva,

SI online Julia L. Monteiro, Arlene G. Corrêa and Márcio W. Paixão





Iron catalyst (10 mol%) 8 h, room temperature





#### **Graphical Abstract**

The cost-effective ferric chloride showed to be an efficient catalyst for the glycosylation of sugars with allyl and alkynyl alcohols, thus leading to the corresponding glycosides in moderate to good yields. Salient features of this simple method include non-hazardous reaction conditions, lowcatalyst loading, good yields and high anomeric selectivity

A Multi-Syringe Flow System for Monitoring Moderately Fast **Chemical Reactions** 

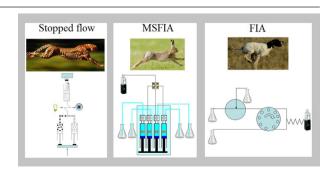
Víctor Cerdà, Carlos Ubide and Juan Zuriarrain

SI online

1989

#### **Graphical Abstract**

The bromine generation and the bromine-salicylic acid reactions have been used for validation of MSFIA in the zone stopping mode. The performance of the technique stays between those of FIA and the classical stopped-flow technique



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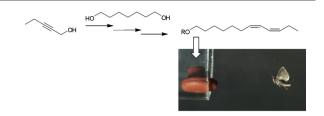
# 1997

#### Synthesis and Field Evaluation of Synthetic Blends of the Sex Pheromone of Crocidosema aporema (Lepidoptera: Tortricidae) in Soybean

SI online Andrés González, Paula Altesor, Leticia Alves, Paola Liberati, Horacio Silva, Juan Ramos, Ignacio Carrera, David González, Gustavo Seoane, Carmen Rossini, Enrique Castiglioni and Daniela Gamenara

#### **Graphical Abstract**

The sex pheromone of the tortricid soybean pest, Crocidosema aporema, was synthesized from 2-pentynol and 1,7-heptanediol, and male captures with different pheromone blends were field-evaluated for the development of pheromone monitoring traps

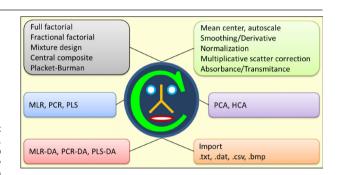


#### 2003 Chemoface: a Novel Free User-Friendly Interface for Chemometrics

Cleiton A. Nunes, Matheus P. Freitas, Ana Carla M. Pinheiro and Sabrina C. Bastos

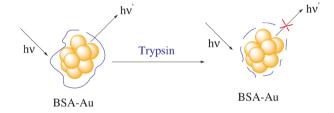
#### **Graphical Abstract**

Chemoface is a free computational tool with user-friendly graphical interface, which is able to work with chemometric methods related to experimental design, pattern recognition, classification and multivariate



#### 2011 A Sensitive Fluorescent Assay for Trypsin Activity in Biological Samples using BSA-Au Nanoclusters

Xianxiang Wang, Yanying Wang, Hanbing Rao and Zhi Shan



### **Graphical Abstract**

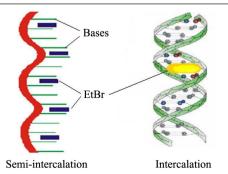
A novel fluorescence analysis method based on trypsin digestion of the protein template of BSA-stabilized Au nanoclusters for sensitive and selective detection of trypsin activity was developed in this work. The methods are utilized potentially for determination of other proteases in clinical diagnostics of various diseases

#### 2016 The Influence of GC/AT Composition on Intercalating and Semi-Intercalating Binding of Ethidium Bromide to DNA

Poghos O. Vardevanyan, Ara P. Antonyan, Marine A. Parsadanyan, Mariam A. Shahinyan, Lilit A. Hambardzumyan, Margarita A. Torosyan and Armen T. Karapetian



Semi-intercalating binding of EtBr occurs along with the ordinary intercalation



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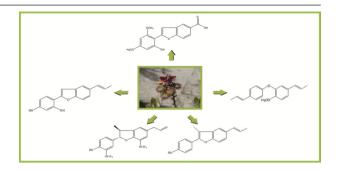
#### 2021 New Neolignans from Krameria tomentosa A. St.-Hil

Sara A. L. Madeiro, Hellane F. S. de Lucena, Caroline D. Siqueira, Marcelo C. Duarte, Raimundo Braz-Filho, José M. Barbosa Filho,

SI online Marcelo S. da Silva and Josean F. Tavares

#### **Graphical Abstract**

Two new neolignans 1,1'-(E)-propenyl-4-methoxy-3,4'-oxyneolignan (ottomentosa) and 5-acid-2-(2'-hydroxy-4',6'-dimethoxyphenyl)benzofuran (sobraline), together with three known neolignans, were isolated from the roots of Krameria tomentosa A. St.-Hil

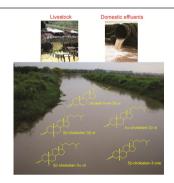


#### 2027 Regional Assessment of Sewage Contamination in Sediments of the Iguaçu and the Barigui Rivers (Curitiba City, Paraná, Southern Brazil) using Fecal Steroids

Lucas Puerari, Renato S. Carreira, Artur C. B. Neto, Lilian C. Albarello and Fabiana D. C. Gallotta

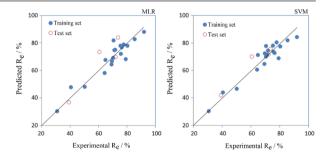
#### **Graphical Abstract**

An evaluation of the contamination by sewage in sediments on a regional scale was performed in the Iguaçu River by considering sterols as indicators. Domestic effluents and manure from rural areas are the main source of contamination. The release of untreated sewage may pose a threat to river health during periods of small river water flow



#### 2035 Prediction of Microdialysis Relative Recovery of Flavone **Derivatives Based on Molecular Descriptors**

Shuyu Zhan, Jianping Huang, Qing Shao, Xiaohui Fan and Wenjing Guo



#### **Graphical Abstract**

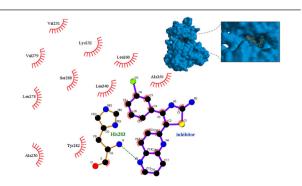
Establish stable and predictive models of multiple linear regression (MLR) and support vector machine (SVM) to predict microdialysis relative recovery of flavone derivatives based on molecular descriptors

#### 2043 Interactions between Activin-Like Kinase 5 (ALK5) Receptor and its Inhibitors and the Construction of a Docking **Descriptor-Based QSAR Model**

Malihe Ebrahimi, Taghi Khayamian and Sajjad Gharaghani

#### **Graphical Abstract**

Docking studies showed that hydrophobic and H-bond interactions are the key factors in the interactions between ALK5 and its inhibitors. Descriptors emerging from docking and molecular structure were used in structure-based QSAR model



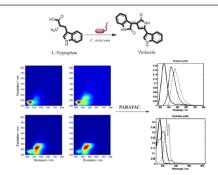
Vol. 23, No. 11, 2012 vii

#### 2054 The Violacein Biosynthesis Monitored by Multi-Wavelength Fluorescence Spectroscopy and by the PARAFAC Method

Clecio Dantas, Pedro L. O. Volpe, Nelson Durán and Márcia M. C. Ferreira

#### **Graphical Abstract**

Combining multi-wavelength fluorescence spectroscopy and the PARAFAC method to link the information obtained from spectral resolution to a biosynthetic pathway

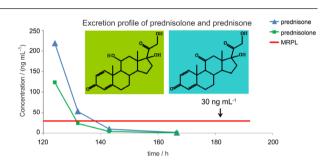


#### 2065 Quantitative Approach to Glucocorticosteroids Analysis in Human Urine using LC-MS/MS

Renata F. Soares, Amanda L. D. de Araújo, Juliana de L. Castro, Luis Nelson L. F. Gomes, Henrique M. G. Pereira and Francisco R. de Aquino Neto

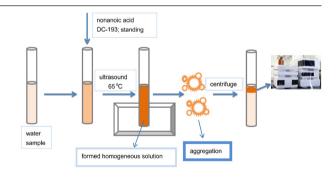
#### **Graphical Abstract**

Urinary excretion profile of prednisolone and prednisone after oral administration of prednisolone. The concentration of 30 ng mL<sup>-1</sup> is the parameter used to establish an adverse analytical finding to exogenous glucocorticosteroids



#### 2075 **Determination of Glucocorticoids using Cosurfactants** Ultrasonic-Thermostatic-Assisted Cloud Point Extraction Followed by High Performance Liquid Chromatography Hui Qin, Gao Feng Li, Nan Chen and Ya Ling Yang

**Graphical Abstract** 2 mL of the solution containing different concentrations of BD, HB and NPP→2.5 mL of DC-193 stock solution and 1mL of nonanoic acid added→standing for 5 min→incubated into ultrasonic-thermostatic bath at 65 °C for 30 min→centrifugation for 3 min at 4000 rpm→achieving a final volume of 0.5 mL by adding acetonitrile→injected into the HPLC

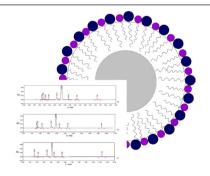


#### 2084 Physicochemical Factors Governing the Partition of Pramipexole and Its Five Impurities in Microemulsion Liquid **Chromatographic Systems**

Ana M. Vemić, Anđelija M. Malenović, Tijana M. Rakić, Nađa M. Kostić, Biljana S. Jančić-Stojanović, Darko P. Ivanović and Mirjana B. Medenica

#### **Graphical Abstract**

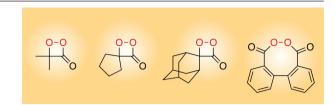
Influences of microemulsion droplet properties and column lipophylicity on partition behavior of pramipexole and its five impurities



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#### 2093 Synthesis of Unstable Cyclic Peroxides for Chemiluminescence

Fernando H. Bartoloni, Marcelo A. de Oliveira, Sl online Felipe A. Augusto, Luiz Francisco M. L. Ciscato, Erick L. Bastos and Wilhelm J. Baader



#### **Graphical Abstract**

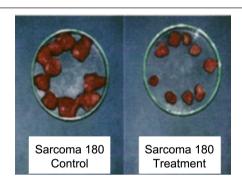
The synthesis, purification and characterization of diphenoyl peroxide and three 1,2-dioxetanones ( $\alpha$ -peroxylactones), important high-energy intermediates in chemi and bioluminescence transformations, are reported

#### 2104 Development and Validation of an LC-UV Method for Quantification of a New Thiazolidinedione (LPSF/AC-23) with Antitumor Activity in Rat Plasma

Raphael D. Valério, Ricardo M. Silva, Hellencléia P. Cunha, Maria C. A. Lima, Suely L. Galdino, Ivan R. Pitta and Maria Bernadete S. Maia

#### **Graphical Abstract**

A quick and simple LC-UV method was developed and validated for quantification of LPSF/AC-23 (CAS No. 675868-75-4), a new antitumor agent in rat plasma. The proposed method can be applied in the quantitative determination of this promising molecule in pharmacokinetic bioavailability studies

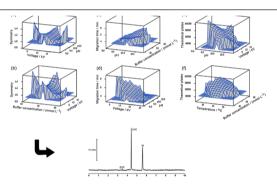


#### Lodenafil Carbonate Tablets: Optimization and Validation of 2114 a Capillary Zone Electrophoresis Method

Cristiane F. Codevilla, Pâmela Cristina L. Ferreira, Maximiliano S. Sangoi, Pedro Eduardo Fröehlich and Ana Maria Bergold

#### **Graphical Abstract**

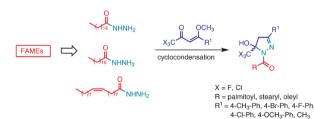
A simple capillary zone electrophoresis method for determination of lodenafil carbonate in drug products was developed and validated. Response surface methodology was used for optimization of the pH and concentration of the buffer, applied voltage and temperature



# **Short Report**

 ${\bf Regiospecific\ Synthesis\ of\ New\ Fatty\ N-Acyl\ Trihalomethylated}$ Pyrazoline Derivatives from Fatty Acid Methyl Esters (FAMEs)

SI online Paulo Beck, Juliane M. dos Santos, Bruna L. Kuhn, Dayse N. Moreira, Alex F. C. Flores, Marcos A. P. Martins, Marcelo G. M. D'Oca and Luciana A. Piovesan



#### **Graphical Abstract**

An efficient and regiospecific route to new fatty N-acyl trihalomethylated pyrazoline derivatives from FAMEs (fatty acid methyl esters) was

2128 An Efficient Synthesis of D-Galactose-Based Multivalent Neoglycoconjugates

**Additions and Corrections** 

Addition related to the article published in Vol. 23, No. 6, 1062-1069, 2012.

2129 Seasonal Distribution of Airborne Trace Elements and Water-Soluble Ions in São Paulo Megacity, Brazil

Addition related to the article published in Vol. 23, No. 10, 1915-1924, 2012.

2130 Flavonoids from the Leaves of *Deguelia utilis* (Leguminosae): Structural Elucidation and Neuroprotective Properties

Addition related to the article published in Vol. 23, No. 10, 1933-1939, 2012.