# 

ISSN 0103-5053

Journal of the Brazilian Chemical Society

Vol. 26, No. 4, April, 2015

# **Cover Picture**



From Caesalpinia pluviosa var. peltophoroides to cytotoxic effect of Caesalpinioflavone in a systematic guide for testing biological activities of novel Natural Products. Details are presented in the Article Caesalpinioflavone, a New Cytotoxic Biflavonoid Isolated from Caesalpinia pluviosa var. peltophoroides by João L. B. Zanin, Murilo Massoni, Marcelo H. dos Santos, Giovana C. de Freitas, Evandro L. O. Niero, Renata R. Schefer, João H. G. Lago, Marisa Ionta and Marisi G. Soares on page 804.

# Contents

# Articles



Novel N-Acylated Benzimidazolone Derivatives: Synthesis, **2D-QSAR and Targets Prediction** Mei and Zhiqin Ji

SI online



Graphical Abstract A series of novel N-acylated benzimidazolone derivatives were synthesized, and their antifungal activity, 2D-quantitative structureactivity relationship (2D-QSAR) and potential targets were studied 642 Fast Classification of Different Oils and Routes Used in Biodiesel Production Using Mid Infrared Spectroscopy and PLS2-DA

Sarmento J. Mazivila, Hery Mitsutake, Felipe B. de Santana, Lucas C. Gontijo, Douglas Q. Santos and Waldomiro Borges Neto

Graphical Abstract Simultaneous classification of type of biodiesels using mid-infrared spectroscopy data and partial least square discriminant analysis (PLS2-DA)



649 HPLC-DAD and UV-Vis Spectrophotometric Methods for Methotrexate Assay in Different Biodegradable Microparticles Alice R. Oliveira, Lilia B. Caland, Edilene G. Oliveira, Eryvaldo S. T. Egito, Matheus F. F. Pedrosa and Arnóbio A. Silva Júnior



High Performance Liquid Chromatography (HPLC) and UV-Vis spectrophotometric methods were developed and validated for analytical quantification of methotrexate (MTX) loaded in biodegradable microparticles produced by the spray-drying technique

660 Main Degradation Products of Dabigatran Etexilate Evaluated by LC-UV and LC-ESI-MS, Degradation Kinetics and *in vitro* Cytotoxicity Studies Raquel M. Bernardi, Felipe B. D'Avila, Vitor Todeschini, Juliana M. M. Andrade, Pedro E. Fröehlich and

Ana M. Bergold

Graphical Abstract Chemical structure of the new oral anticoagulant dabigatran etexilate (DAB) and proposed structures of their degradation products

> LEIS SVET OM SET UP WELD METAL BASE



## Graphical Abstract

**Graphical Abstract** 

Comparative analysis of three techniques: localized electrochemical impedance spectroscopy (LEIS), technique of scanning vibrating electrode (SVET) and optical microscopy (OM) applied to the experimental setup carbon steel (base) and carbon steel subjected to tungsten inert gas (TIG) weld. Analysis after 2 h with electrodes electrically connected immersed in NaCl 0.05 mol L<sup>-1</sup>



Application of Headspace Solid-Phase Microextraction and Gas Chromatography-Mass Spectrometry (HS-SPME-GC/ MS) on the Evaluation of Degradation Efficiency of Phenolic SI online Compounds and Identification of By-Products from Produced Water

Cesar A. Silva and Luiz A. S. Madureira

**Graphical Abstract** Determination of phenols in produced water and possible generated by-products formed during photochemical degradation processes by HS-SPME-GC/MS. Optimum experimental conditions enabled degradation of more than 99% of the initial concentrations of the total phenolic components of produced water









Can Ergosterol Be an Indicator of Fusarium Fungi and **Mycotoxins in Cereal Products?** 

Ewa Stanisz, Agnieszka Zgoła-Grześkowiak, Agnieszka Waśkiewicz, Łukasz Stępień and Monika Beszterda SI online

> **Graphical Abstract** Determination of ergosterol as indicator of fungal contamination and selected mycotoxins was done in several samples of grain products to examine existence of possible correlations between these compounds. Fungi responsible for contamination were also identified





Simultaneous Determination of Ascorbic Acid, L-Dopa, Uric Acid, Insulin, and Acetylsalicylic Acid on Reactive Blue 19 and Multi-Wall Carbon Nanotube Modified Glassy Carbon Electrode SI online

Navid Nasirizadeh, Zahra Shekari, Masoumeh Tabatabaee and Masoud Ghaani

## Graphical Abstract

A new trifunctional sensor, based on a reactive blue 19 and multi-wall carbon nanotube modified glassy carbon electrode (RB-MWCNT-GCE), was constructed. RB-MWCNT-GCE was applied for simultaneous determination of ascorbic acid (AA), levodopa (LD), uric acid (UA), insulin, and acetylsalicylic acid (ASA) in mixture



723 Virginicin, a New Naphthalene from Kosteletzkya virginica (Malvaceae) Bai Bai, Xu-Wei Gu, Yu Chen, Fu-Qin Guan, Yu Shan and

SI online Xu Feng

## **Graphical Abstract**

A new naphthalene, 8-methoxy-2,7-dihydroxyl-4-(1'-hydroxyl-isopropyl)-6-methyl-1-naphthaldehyde was isolated from the tubers of Kosteletzkya virginica. It was evaluated for its potential in scavenging diphenylpicryl hydrazyl radical (DPPH<sup>•</sup>), inhibition of nitric oxide (NO) induced by lipopolysaccharide (LPS), cytotoxic activity against human acute promyelocytic leukemia (HL-60) and human colorectal adenocarcinoma (LOVO) cell lines



729 Development and Validation of a Dissolution Test Method for Albendazole and Praziquantel in Their Combined Dosage Form Silvana E. Vignaduzzo, María A. Operto and Patricia M. Castellano

> **Graphical Abstract** This study aimed to develop a dissolution test for tablets containing albendazole and praziquantel for veterinary use





Cytotoxic Chalcones from Desmodium oxyphyllum Xue-Mei Gao, Huan Wang, Yin-Ke Li, Bing-Kun Ji, Cong-Fang 【 Xia, Juan-Xia Yang, Min Zhou, Yan-Qing Ye and Qiu-Fen Hu

SI online



 $R^1 = OH, R^2 = H, R^3 = OMe$  $R^1 = OMe, R^2 = H, R^3 = OH$  $R^1 = OH, R^2 = OH, R^3 = OMe$ 

**Graphical Abstract** Three new chalcones isolated from Desmodium oxyphyllum

## Vol. 26, No. 4, 2015



A method for obtaining biarylic units from tyrosine derivatives via Suzuki-Miyaura cross-coupling using a variety of potassium aryltrifluoroborate salts



Graphical Abstract

Validation of a high performance liquid chromatography (HPLC) method for aflatoxins determination in corn arepas commercialized in Manizales, Colombia





Caesalpinioflavone, a New Cytotoxic Biflavonoid Isolated from Caesalpinia pluviosa var. peltophoroides

João L. B. Zanin, Murilo Massoni, Marcelo H. dos Santos,
Sl online Giovana C. de Freitas, Evandro L. O. Niero, Renata R. Schefer,
João H. G. Lago, Marisa Ionta and Marisi G. Soares



Graphical Abstract Caesalpinioflavone, a novel biflavonoid isolated from Caesalpinia pluviosa var. peltophoroides, displays antitumor potential against A549, MCF7, Hs578T and HTC cell lines

## **Short Reports**



SI online Diogo S. Lüdtke



### Graphical Abstract

The synthesis of alkylseleno carbohydrates starting from different sugar scaffolds is described. The synthesized molecules had their antioxidant activity profile evaluated and promising results were found for one of the synthesized compounds

816A New Straightforward Synthesis of 2', 3'-Didehydro-2',<br/>3'-dideoxy-2'-(2''-(trimethylsilyl)ethylthio)thymidine,<br/>Key Intermediate for the Synthesis of 2'-Substituted

SI online **Thionucleosides** Maralise P. Olive

Maralise P. Oliveira, Lucas L. Franco, Maria C. A. Lima, Cláudia M. O. Simões, Suely L. Galdino, Ivan R. Pitta, Jean-Luc Décout and Ricardo J. Alves

### Graphical Abstract

Short and efficient synthesis of 2',3'-didehydro-2',3'-dideoxy-2'-(2''-(trimethylsilyl)ethylthio)thymidine which allows the preparation of diverse potentially antiviral and/or anticancer nucleosides

822 Collision-Induced Dissociation Analysis of Brevianamide A and C in Electrospray Ionization Mass Spectrometry Ana Lígia L. de Oliveira, Ricardo Vessecchi, Norberto P. Lopes and Hosana M. Debonsi

> Graphical Abstract Computational chemistry and collision-induced dissociation analysis of brevianamide A and C allow discrimination between isomeric cyclic peptides isolated from *Penicillium brevicompactum* and sheds light on diketopiperazine fragmentation mechanisms





# **Additions and Corrections**

828	Validation of the Determination of Fatty Acids in Milk by Gas
	Chromatography
	Julliana Isabelle Simionato, Juliana Carla Garcia,
	Geraldo Tadeu dos Santos, Cláudio Celestino Oliveira.

Jesui Vergilio Visentainer and Nilson Evelázio de Souza

829 Quantification of Harman Alkaloids in Sour Passion Fruit Pulp and Seeds by a Novel Dual SBSE-LC/Flu (Stir Bar Sorptive Extraction - Liquid Chromatography with Fluorescence Detector) Method Cíntia A. M. Pereira, Thyago R. Rodrigues and Janete H. Yariwake Addition related to the article published in Vol. 21, No. 3, 520-524, 2010.

Addition related to the article published in Vol. 25, No. 8, 1472-1483, 2014.