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Cover Picture



The number of petals on a flower can be key to its taxonomy and properties, so too the number of thiophenyl groups on a corannulene imbue it with color, radiance and (electron) attractiveness. Each phenylthio derivative (n = 0-10) presents like a flower in a bouquet, assembling a veritable anthology of aromatics. Stemming from this chemical florilegium are principle additivity parameters useful for predicting the character of future corannulene-based inflorescence. Details are presented in the Article **Tunable Photochemical/Redox Properties of (Phenylthio)**_ncorannulenes: Application to a Photovoltaic **Device** by *Angela Steinauer, Anna M. Butterfield, Anthony Linden, Agustin Molina-Ontario, David C. Buck, Robert W. Cotta, Luis Echegoyen, Kim K. Baldridge, and Jay S. Siegel* on page 1866.

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Editorial

1705 It Is Necessary to Resist Aldo José Gorgatti Zarbin

The rest of the molecule

Analytical curve without preconcentration

003 + 0.01357fCd2+

300 400

FAAS

Articles

1706

Preparation of Two Maleic Acid Sulfonamide Salts and Their Copper(II) Complexes and Antiglaucoma Activity Studies Cengiz Yenikaya, Halil İlkimen, Mehmet Melih Demirel,

SI online Burçin Ceyhan, Metin Bülbül and Ekrem Tunca

Graphical Abstract Two proton transfer salts and three copper(II) complexes have been synthesized and their antiglaucoma activities were studied *in vitro*.

1715 Solid Phase Extraction to On-Line Preconcentrate Trace Cadmium Using Chemically Modified Nano-Carbon Black with 3-Mercaptopropyltrimethoxysilane

Caroline D. Zappielo, Daniel M. Nanicuacua, Walter N. L. dos Santos, Daniel L. F. da Silva, Luiz H. Dall'Antônia, Fernanda M. de Oliveira, Débora N. Clausen and César R. T. Tarley

Graphical Abstract

Eluen

Modified carbon black was used as an alternative nano-carbonaceous material for the preconcentration of trace levels of Cd²⁺ in different samples with posterior determination by flame atomic absorption spectrometry (FAAS).

1727 Effects of Different Numbers of Fungicide Application on the Proximate Composition of Soybean Roger N. Michels, Elton G. Bonafe, Luana C. Figueiredo, Rúbia M. Suzuki, Lilian D. Tonin, Paula F. Montanher,

> Alessandro Francisco Martins, Jesui V. Visentainer, Marcelo G. Canteri and Marcelo Augusto A. Silva

> > Graphical Abstract

Concentration evaluated of many compounds such as phytosterols, tocopherols, fatty acids and antioxidant, after different applications of fungicides.



1736 The HPLC Fingerprint Analysis of Selected *Cirsium* Species with Aid of Chemometrics

Anna M. Hawrył, Agata Ziobro, Ryszard S. Swieboda, Mirosław A. Hawrył, Mykhaylo Chernetskyy and Monika Waksmundzka-Hajnos

Graphical Abstract

Twelve *Cirsium* sp. methanolic extracts were analyzed using highperformance liquid chromatography to construct the appropriate fingerprint chromatograms. Obtained chromatograms were compared using various similarity and distance indices and the obtained results were compiled using principal component analysis (PCA).



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 1744 Ibuprofen, Carbamazepine and β-Estradiol Determination Using Thin-Film Microextraction and Gas Chromatography-Mass Spectrometry Ady Giordano, José Vásquez, Mauricio Retamal and Loreto Ascar

> Graphical Abstract Thin-film extraction procedure used for the determination of selected compounds from water samples.



Estuary Adjacent to a Megalopolis as Potential Disrupter of Carbon and Nutrient Budgets in the Coastal Ocean Letícia Lazzari, Angela L. R. Wagener, Cássia O. Farias,

Sl online Aída P. Baêta, Cristiane R. Mauad, Alexandre M. Fernandes, Rodolfo Paranhos and Renato S. Carreira

Graphical Abstract Organic carbon (OC), N and P daily flow rates from Guanabara Bay to coastal ocean were obtained. Estimated OC, N and P flow rates are regionally and globally significant. Carbon (δ¹³C) and nitrogen (δ¹⁵N) isotopic composition and sterols reveal export of labile carbon, thus, of high nutritive value. The photo was taken during sampling.



1766 Phosphate Modification of Nano Titania and Its Effect on the Photodegradation of EDTA Effat Iravani, Sareh Ammari Allahyari and

SI online Meisam Torab-Mostaedi

Graphical Abstract

Efficiency and kinetic of ethylenediaminetetraacetic acid disodium salt (EDTA) degradation showed considerable performance in the presence of phosphate modified nano titania compared to untreated nano titania probably due to better EDTA adsorption.





Rafał Giszter, Marta Fryder, Katarzyna Marcinkowska and Sl online Agata Sznajdrowska



Graphical Abstract Herbicidal ionic liquids tend to prevent drops from running off the leaf and improve the wettability. Increasing time of contact with the surface of the leaves has a positive influence on the herbicide formulation efficacy.

1782 Application of an Accurate and Validated Method for Identification and Quantification of Acrylamide in Bread, Biscuits and Other Bakery Products Using GC-MS/MS System Mioara Negoiță and Alina Culețu



Graphical Abstract Separation, detection, identification and guantification of acrylamide.

1792 Application of Solvent Demulsification-Dispersive Liquid-Liquid Microextraction Based on Solidification of Floating Organic Drop Coupled with High Perfomence Liquid Chromatography in Determination of Sulfonylurea Herbicides in Water and Soil

Li Yan, Zhu Jing, Ren Lin, Li Yongxin and Zou Xiaoli

Graphical Abstract

SD-SFO-DLLME (solvent-based demulsification and solidification of a floating organic drop combined with dispersive liquid-liquid microextraction): extractant and dispersing reagent were injected into the sample solution to extract the target compounds for HPLC-UV (high performance liquid chromatography with ultraviolet detection) analysis.



Evaluating the "Tape Tea" Myth as Low Cost Abuse Drug 1800 through Mass Spectrometry Eraldo L. Lehmann, Deleon N. Correa, Eduardo M. Schmidt, Marcos N. Eberlin and Marco A. Z. Arruda

Graphical Abstract This graphical abstract summarizes the dangers of drinking "tape tea" due to the presence of neurotoxic and carcinogenic elements.



Synthesis and Antifungal Activity Against Candida Strains of Mesoionic System Derived From 1,3-Thyazolium-5-thiolate Isabelle N. Peixoto, Helivaldo D. S. Souza, Bruno F. Lira, Sl online Daniele F. Silva, Edeltrudes O. Lima, José M. Barbosa-Filho and Petrônio F. de Athayde-Filho



Tape tea

Graphical Abstract

Ten new mesoionic derivatives from the 1.3-thiazolium-5-thiolate system with substituted acetamides were synthesized, had their potential as new drug evaluated in an in silico study and in their activity as antifungal against strains of Candida albicans.



1847 **Electrochromic Properties of Polyaniline-Based Hybrid Organic/Inorganic Materials** Rosanny C. Silva, Marina V. Sarmento, Roselena Faez,

Roger J. Mortimer and Adriana S. Ribeiro





clay(-) films

PAni-clay chromaticity coordinates

Graphical Abstract This scheme summarises the spectroelectrochemical results obtained for the samples of the hybrid materials based on polyaniline, chitosan and/or an organically modified clay.

1858 A Study of the Interaction Between trans-Dehydrocrotonin, a Bioactive Natural 19-nor-Clerodane, and Serum Albumin Otávio Augusto Chaves, Breno A. Soares, Maria Aparecida M. Maciel, Carlos Maurício R. Sant'Anna, José Carlos Netto-Ferreira, Dari Cesarin-Sobrinho and Aurélio B. B. Ferreira



Graphical Abstract The binding between serum albumin and the bioactive 19-nor-clerodane trans-dehydrocrotonin (t-DCTN) is weak and essentially due to hydrophobic interactions.



Tunable Photochemical/Redox Properties of (Phenylthio), corannulenes: Application to a Photovoltaic Device Angela Steinauer, Anna M. Butterfield, Anthony Linden, Slonline Agustin Molina-Ontario, David C. Buck, Robert W. Cotta, Luis Echegoyen, Kim K. Baldridge and Jay S. Siegel

Graphical Abstract

The additive substituent effect of phenylmercaptoderivatives of corannulene are investigated by spectroscopic and electrochemical techniques. The per-substituted phenylmercaptocorannulene is incorporated as a replacement for [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) in a photovoltaic device.





Chemical Profile and Cytotoxic Activity of Leaf Extracts from Senna spp. from Northeast of Brazil

Juliana G. A. Silva, Alexander A. Silva, Isabel D. Coutinho, Sl online Claudia O. Pessoa, Alberto J. Cavalheiro and Maria G. V. Silva

Graphical Abstract

Using dereplication, gas chromatography coupled to mass spectrometry (GC-MS) and multivariate analyses by hierarchical cluster analysis (HCA) and partial least squares-discriminant analysis (PLS-DA), of 12 extracts from four Senna spp., hit compounds were identified and the steps of extract fractionation and purification of known compounds were avoided; therefore, in the prospect for new drug prototypes from biological sources, the research approach was improved.



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Ethanol Production from Sugarcane Bagasse Using Phosphoric Acid-Catalyzed Steam Explosion Ana Paula Pitarelo, César S. da Fonseca, Luana M. Chiarello,

SI online Francisco M. Gírio and Luiz P. Ramos

Graphical Abstract

Steam explosion with or without dilute phosphoric acid resulted in a good pretreatment performance of cane bagasse. High hydrolysis and fermentation yields were obtained from water-washed steam-treated substrates but the pretreatment water solubles were highly inhibitory. Freeze-drying water-soluble furan compounds and acetic acid to non-inhibitory levels.



1899 Chromophoreasy, an Excel-Based Program for Detection and Integration of Peaks from Chromatographic and Electromigration Techniques

SI online Fernando A. S. Vaz, Leandra N. O. Neves, Rafael Marques, Renata T. Sato and Marcone A. L. Oliveira



Graphical Abstract Overview of Chromophoreasy: a simple, practical and reliable program that detects and integrates chromatographic and electrophoretic peaks.

Short Reports _



Dayane A. Santos, Karen P. Lima, Paulo H. Março and Sl online Patrícia Valderrama



Graphical Abstract A multiproduct calibration based on ultraviolet spectroscopy and Tillman's titration as reference method was developed to predict vitamin C in industrialized juices.



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