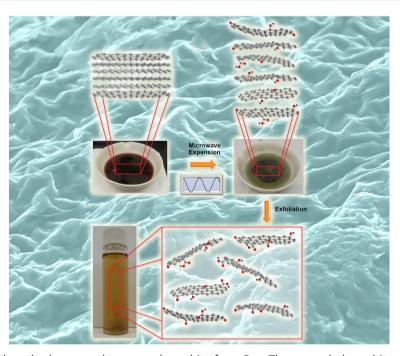
Journal of the Brazilian Chemical Society

ISSN 0103-5053

Vol. 26, No. 5, May, 2015

Cover Picture



Microwave-assisted acid method was used to expand graphite from Bay. The expanded graphite obtained was sonicated in acid medium to prepare wrinkled 2Dfew-layered graphene oxide with 5 to 9 layers that showed good stability in water from pH 4 to 12. The global process is a fast and energy-saving method compared to other processes described in the literature. Details are presented in the Article Facile Graphene Oxide Preparation by Microwave-Assisted Acid Method by Marcelo M. Viana, Meiriane C. F. S. Lima, Jerimiah C. Forsythe, Varun S. Gangoli, Minjung Cho, Yinhong Cheng, Glaura G. Silva, Michael S. Wong and Vinicius Caliman on page 978.

Contents

Editorial

iv J. Braz. Chem. Soc.

Communication

Solventless and Mild Procedure to Prepare Organotellurium(IV) 832 **Compounds under Microwave Irradiation**



Cleverson Princival, Alcindo A. Dos Santos and João V. Comasseto



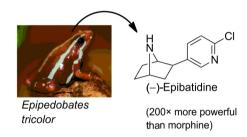
Graphical Abstract

p-Methoxyphenyltellurium trichloride reacts with alkynes in a short reaction time under microwave irradiation in the absence of solvents

Review

Recent Syntheses of Frog Alkaloid Epibatidine

Ronaldo E. de Oliveira Filho and Alvaro T. Omori



Graphical Abstract

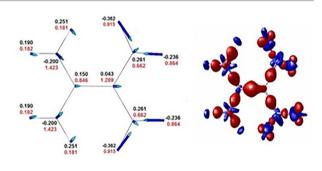
This review presents the recent syntheses of epibatidine since 2002, summarized by the method used to obtain the azabicyclic core

Articles

Molecular Electronic Topology and Fragmentation Onset via Charge Partition Methods and Nuclear Fukui Functions: 1,1-Diamino-2,2-dinitroethylene

SI online

Tiago Giannerini and Itamar Borges Jr.



Graphical Abstract

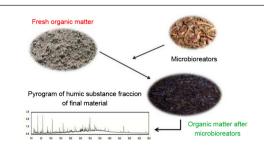
Topological methods and response functions were used to investigate in detail the electronic (charge) properties of 1,1-diamino-2,2dinitroethylene (FOX-7) including acid-base properties and onset of fragmentation

860 Chemical Differentiation of Domestic Sewage Sludge and Cattle Manure Stabilized by Microbioreators: Study by Pyrolysis Coupled to Gas Chromatography Coupled to Mass Spectroscopy

Paulo R. Dores-Silva, Maria D. Landgraf and Maria O. O. Rezende

Graphical Abstract

The earthworms act as microbioreactors leading to various several unit operations that conduce the stabilization of the recent organic matter, transforming it in a more refratory material



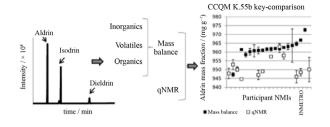
Vol. 26, No. 5, 2015

869 Determination of Aldrin Purity Using a Combination of the Mass Balance Approach and Quantitative NMR

Janaína M. Rodrigues, Eliane C. P. Rego, Evelyn F. Guimarães, Marcus V. B. Sousa, Tânia M. Monteiro, Laura A. Neves, Fernando G. M. Violante, Renato R. R. Almeida, Maria C. B. Quaresma and Raquel Nogueira

Graphical Abstract

Aldrin mass fraction was determined by mass balance, after determination of impurity mass fractions by gas chromatography with flame ionization detection, gas chromatography-mass spectrometry, gas chromatography with electron capture detector (organics), Karl Fischer coulometric titration (water content), and inductively coupled plasma mass spectrometry (inorganics). The results were validated through the participation of the National Institute of Metrology, Quality and Technology in the key-comparison CCQM-K55.b organized by Organic Analysis Working Group/International Bureau of Weights and Measures

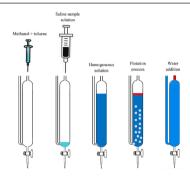


880 Extraction and Separation of Molybdenum by Using Homogeneous Liquid-Liquid Microextraction via Flotation

Mohammad Rezaee, Maryam Mozaffari, Hedayat Haddadi, Mohammad R. Pourjavid and Abolfazl Semnani

Graphical Abstract

Homogeneous liquid-liquid microextraction via flotation assistance was investigated for the extraction of molybdenum from water samples. The developed method was sensitive, reproducible and linear over a wide range



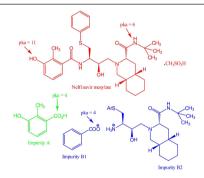
887

Optimization of an Electrolyte System for the Simultaneous Separation of Nelfinavir Mesylate and Two Impurities by Micellar Electrokinetic Chromatography

SI online Carina A. Bastos, Cláudia R. B. Gomes, Marcus V. N. de Souza and Marcone A. L. de Oliveira

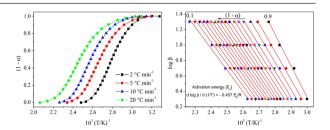
Graphical Abstract

A methodology for the determination of nelfinavir and its impurities was proposed using micellar electrokinetic chromatography (MEKC)-UV. The electrolyte was optimized using mixed-level factorial design. The robustness (using Youden's test) showed that the buffer concentration had the greatest effect in the separation factor



899 Kinetic Investigation of Thermal Formation Processes of SiOC Glasses Derived from C-Containing Hybrid Polymeric Networks

Naiara V. Godoy and Mariana G. Segatelli SI online



Graphical Abstract

The activation energies (E_a) of the thermal degradation processes in C-rich and poor SiOC glasses, determinated by Ozawa method, allowed to identify two degradation steps for all samples with different complexities

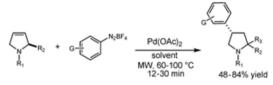
J. Braz. Chem. Soc. vi



Microwave-Assisted Heck Arylations of Non-Activated N-Acyl-3-pyrrolines with Arenediazonium Tetrafluoroborates

Fernanda G. Finelli, Marla N. Godoi and

SI online Carlos R. D. Correia



R ₁	R ₂	R ₃	G	Conventional heating		Microwave	
				time	Yield	time	Yield
Boc	н	ОН	4-OMe	30 min	15%	15 min	84%
CO ₂ Me	CO ₂ Me	OMe	4-OMe	18 h	86%	12 min	84%
CO ₂ Me	CO₂Me	OMe	4-F	18 h	55%	15 min	48%

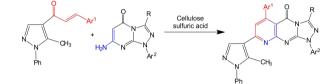
Graphical Abstract

Effective Heck arylations of non-activated N-acyl-3-pyrrolines with arenediazonium salts were accomplished applying microwave irradiation

916

Cellulose Sulfuric Acid as an Eco-Friendly Catalyst for Novel Synthesis of Pyrido[2,3-d][1,2,4]triazolo[4,3-a]pyrimidin-5-

Sobhi M. Gomha and Sayed M. Riyadh



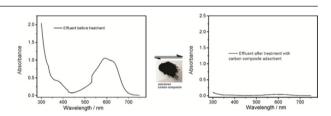
Graphical Abstract

In the present work, novel procedure for synthesis of pyrido[2,3-d][1,2,4] triazolo[4,3-a] pyrimidin-5-ones has been reported by using cellulose sulfuric acid as biopolymeric solid support acid catalyst

924

Application of Carbon Composite Adsorbents Prepared from Coffee Waste and Clay for the Removal of Reactive Dyes from Aqueous Solutions

SI online Davis C. dos Santos, Matthew A. Adebayo, Eder C. Lima, Simone F. P. Pereira, Renato Cataluña, Caroline Saucier, Pascal S. Thue and Fernando M. Machado



Graphical Abstract

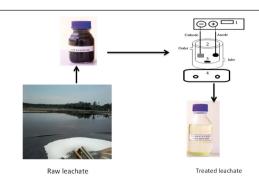
Dye-contaminated effluent treated with carbon composite adsorbent. Left untreated effluent, right treated effluent

939 Electrochemical Oxidation of Landfill Leachate: Investigation of Operational Parameters and Kinetics Using Graphite-PVC Composite Electrode as Anode

Zainab H. Mussa, Mohamed R. Othman and Md P. Abdullah

Graphical Abstract

Raw leachate is a complicated sample with high chemical oxygen demand (COD) and color. Hence, a cheap, effective, and easy electrochemical oxidation technique is used in this study to reduce the concentration of pollutants in terms of COD and color



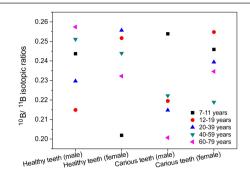
Vol. 26, No. 5, 2015

949 Determination of Boron Isotope Ratios in Tooth Enamel by Inductively Coupled Plasma Mass Spectrometry (ICP-MS)

After Matrix Separation by Ion Exchange Chromatography Maoyong He, Zhangdong Jin, Chongguang Luo, Li Deng, Jun Xiao and Fei Zhang

Graphical Abstract

The 10 B/ 11 B ratio in the enamel of the healthy teeth and carious teeth fluctuated over a broad range, ranged from 0.2007 to 0.2574. And it has significant variation with respect to age and gender



955

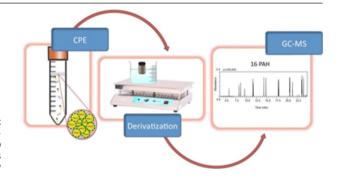
Determination of Polycyclic Aromatic Hydrocarbons in Groundwater Samples by Gas Chromatography-Mass Spectrometry After Pre-Concentration Using Cloud-Point Extraction with Surfactant Derivatization

SI online

Sarah A. R. Soares, Cibele R. Costa, Rennan G. O. Araujo, Maria R. Zucchi, Joil J. Celino and Leonardo S. G. Teixeira

Graphical Abstract

A cloud-point extraction method using the surfactant (30)*p-tert*octylphenol polyoxyethylene was proposed as the preceding step
for the determination of polycyclic aromatic hydrocarbons by gas
chromatography-mass spectrometry

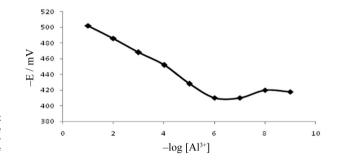


963 Construction of a New Aluminum(III) Cation Selective Electrode Based on 12-Crown-4 as an Ionophore

Masoomeh Esmaelpourfarkhani, Gholam H. Rounaghi and Mohammad H. Arbab-Zavar

Graphical Abstract

The macrocyclic ligand, 12-crown-4, was used as an ionophore for fabrication of a polyvinyl chloride based membrane sensor for aluminum(III) cation. It was successfully used for the determination of this metal cation in some rocks and aluminum-magnesium syrup



970

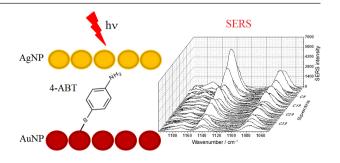
Intercalated 4-Aminobenzenethiol between Au and Ag Nanoparticles: Effects of Concentration and Nanoparticles Neighborhood on its SERS Response

SI online

Elias de Barros Santos, Fernando Aparecido Sigoli and Italo Odone Mazali

Graphical Abstract

Intercalated 4-aminobenzenethiol between gold and silver nanoparticles was prepared and its surface-enhanced Raman scattering (SERS) signal is dependent on sandwiched nanostructure



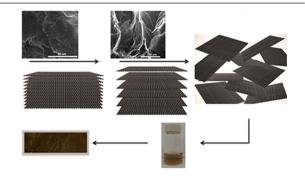
viii J. Braz. Chem. Soc.

978 Facile Graphene Oxide Preparation by Microwave-Assisted Acid Method

Marcelo M. Viana, Meiriane C. F. S. Lima, Jerimiah C. Forsythe, Varun S. Gangoli, Minjung Cho, Yinhong Cheng, Glaura G. Silva, Michael S. Wong and Vinicius Caliman

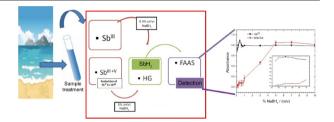
Graphical Abstract

Expansion, exfoliation and oxidation of graphite using a microwaveassisted acid method to prepare few layers graphene oxide (GO) and reduced graphene oxide (rGO) film with relatively high electrical conductivity



985 Noteworthy Method for Direct Determination of Sb^{III} and Total Inorganic Antimony in Natural Waters

Thaís S. Neri, Dayene C. Carvalho, Vanessa N. Alves and Nívia M. M. Coelho



Graphical Abstract

A procedure was developed for the direct determination of Sb^{III} and total inorganic Sb in water samples by hydride generation atomic absorption spectrometry (HG AAS), without pre-reduction of Sb^V

992 New Flexible and Transparent Solution-Based Germanium-Sulfide Polymeric Materials

Denise T. B. De Salvi, Aldo E. Job and Sidney J. L. Ribeiro

Ged. 1.3-propanedithiol Ged. 1.3-propanedithiol Ged. 1.3-propanedithiol Ged. 1.3-propanedithiol Ged. 1.3-propanedithiol Ged. 1.3-propaned Ged. 1.3-propaned

Graphical Abstract

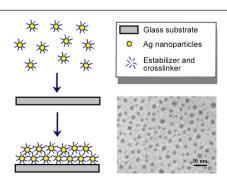
These polymers present germanium and sulfur in their structure. They are transparent in the visible range and show flexibility. Other characteristic is the glass transition temperature found in temperatures below 0 °C, which may suggest applications in low temperatures

1004 Silver Nanoparticle Thin Films Deposited on Glass Surface Using an Ionic Silsesquioxane as Stabilizer and as Crosslinking Agent

Andressa C. Schneid, Marcelo B. Pereira, Flavio Horowitz, Raquel S. Mauler, Carla R. Matte, Manuela P. Klein, Plinho F. Hertz, Tania M. H. Costa, Eliana W. de Menezes and Edilson V. Benvenutti

Graphical Abstract

One step deposition of thin films containing silver nanoparticles on glass surfaces was made using charged silsesquioxane as nanoparticle stabilizer and as crosslinking agent. The system showed antimicrobial activity and it is promising as coating for glass used as food package and for hospital instruments that require sterilization



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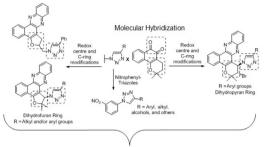
1013

On the Search for Potential Antimycobacterial Drugs: Synthesis of Naphthoquinoidal, Phenazinic and 1,2,3-Triazolic Compounds and Evaluation Against Mycobacterium tuberculosis

SI online Guilherme A. M. Jardim, Eduardo H. G. Cruz, Wagner O. Valença, Jarbas M. Resende, Bernardo L. Rodrigues, Daniela F. Ramos, Ronaldo N. Oliveira, Pedro E. A. Silva and Eufrânio N. da Silva Júnior

Graphical Abstract

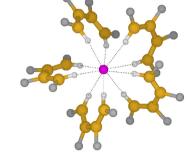
The present study describes the synthesis of naphthoguinoidal derivatives, phenazines and aryl triazoles as well as the evaluation of these compounds against Mycobacterium tuberculosis. This report represents an important contribution to the discovery of new anti-tuberculosis derivatives



All compounds evaluated against Mycobacterium tuberculosis

1028 Theoretical Study of Molecular and Electronic Structures of 5, Knot Systems: Two-Layered ONIOM Calculations

Aguinaldo R. de Souza and Nelson H. Morgon



Graphical Abstract

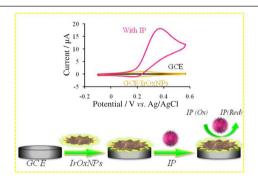
Theoretical study of the molecular fragment present in the experimental structure of the [5₁ knot×××(PF₆)₉]Cl system using ONIOM(M06/6-31G(2d,p):PM6) method

1034 Amperometric Detection of Isoprenaline Based on Glassy Carbon Electrode Modified by Iridium Oxide Nanoparticles

Mahmoud Roushani and Somayeh Farokhi

Graphical Abstract

A simple and very sensitive electrochemical sensor based on iridium oxide nanoparticles (IrOxNPs) has been developed by modification of glassy carbon electrode (GCE) and utilized to determine isoprenaline (IP). This sensor was used successfully for IP determination in human urine samples. The detection limit of the modified electrode toward IP was 90 nmol L-1



1043

Biotransformation of the Diterpene Ent-18,19dihydroxytrachylobane by Rhizopus stolonifer

SI online

Daniely H. P. Vasconcelos, Jair Mafezoli, Paula K. S. Uchôa, Natalia N. Saraiva, Mary A. S. Lima, José N. Silva Júnior, Francisco G. Barbosa, Marcos C. Mattos, Maria C. F. de Oliveira, Cristiano S. Lima and Maria N. G. Pessoa

Graphical Abstract

The diterpene ent-18,19-dihydroxytrachylobane was biotransformed by Rhizopus stolonifer, and yielded three new compounds: ent-118,18,19trihydroxytrachylobane, ent-16a,18,19-trihydroxykaur-11-ene and ent-18,19-dihydroxy-16a-methoxykaur-11-ene



J. Braz. Chem. Soc.

Short Reports ____

1048 Fluorescence Quenching of Two meso-Substituted Tetramethyl BODIPY Dyes by Fe(III) Cation
Lucas C. D. Rezende and Flavio S. Emery

SI online

Fluorescence turn-off

Graphical Abstract

Chemical structures of the main borodiazaindacenes (BODIPYs) and the fluorescence turn-off observed under black light for the pyridyl-substituted BODIPY with growing concentration of Fe(III)