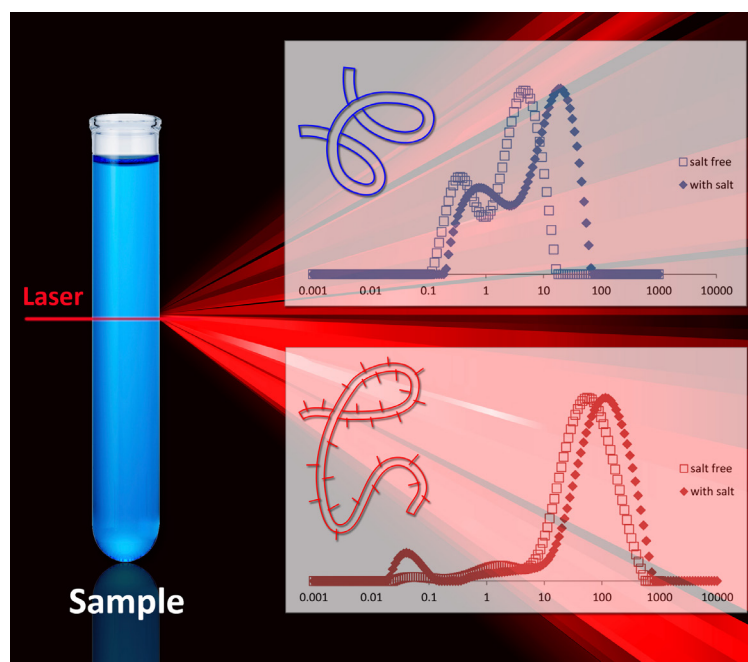


Cover Picture



The pattern of light scattering may be used to identify inter and intramolecular interactions of macromolecules, such as polymers. However, when there are more than one relaxation mode its interpretation is not always easy, and may lead to misunderstandings. This is the case of hydrophobically modified polyacrylamides, with or without charges. Details are presented in the Article **Polyelectrolyte and Non-Polyelectrolyte Polyacrylamide Copolymers Solutions: the Role of Salt on the Intra- and Intermolecular Interactions** by Ana M. S. Maia, Marcos A. Villetti, RedouaneBorsali and Rosangela C. Balaban on page 1871.

Contents

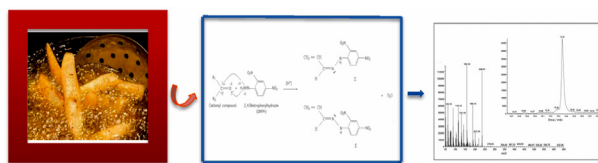
Editorial

1707 A New Era of SBQ Publications
Editors of JBCS and Química Nova

Review

1711 Analytical Methods to Assess Carbonyl Compounds in Foods and Beverages

Vanessa M. Osório and Zenilda L. Cardeal



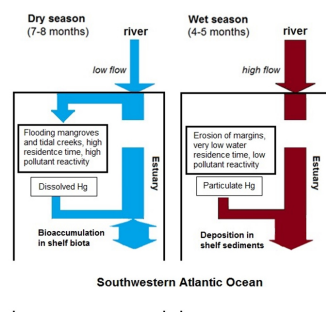
Graphical Abstract

Carbonyl compounds are widely found in food products such as fried food. A derivatizing agent (2,4-dinitrophenylhydrazine) in conjunction with a chromatographic mass spectrometry system is the usual method to assess carbonyl compounds in foods and beverages

Articles

1719 Pluriannual Watershed Discharges of Hg into a Tropical Semi-Arid Estuary of the Jaguaribe River, NE Brazil

Luiz D. Lacerda, Francisco J. S. Dias, Rozane V. Marins, Talita M. Soares, José Marcos O. Godoy and Maria Luíza D. P. Godoy

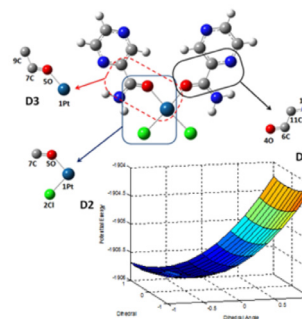


Graphical Abstract

Estuarine hydrodynamics under semiarid climate and the effects on Hg export to the sea in the Jaguaribe Estuary, NE Brazil

1732 A Computational Study of the Complex Dichlorobis(pyrazinamido)platinum(II), [PtCl₂(PZA)₂], Applying a Mixed-Level Factorial Design

Paola Araujo S. Oliveira, Lucas M. Sartori, Nicolás A. Rey, Hélio F. Dos Santos, Marcone Augusto L. De Oliveira and Luiz Antônio S. Costa

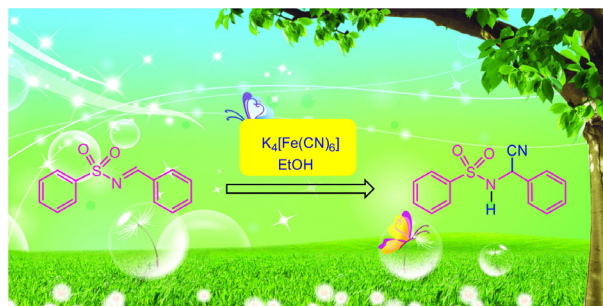


Graphical Abstract

A computational search (DFT) for the most stable structure of Pt(II)-PZA complex was performed associated to a mixed-level factorial design (5x3). Such statistical scheme allowed us to optimize system stability and interaction effects, among others

1739 Hydrocyanation of Sulfonylimines Using Potassium Hexacyanoferrate(II) as an Eco-Friendly Cyanide Source

Zheng Li, Rongzhi Li, Huanhuan Zheng, Fei Wen, Hongbo Li, Junjun Yin and Jingya Yang



Graphical Abstract

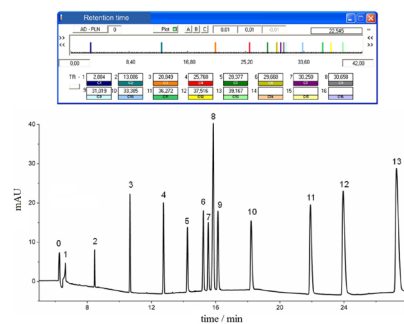
An eco-friendly hydrocyanation method for sulfonylimines using non-toxic, nonvolatile and inexpensive potassium hexacyanoferrate(II) as an original cyanide source has been developed

1744 Optimization of Electrophoretic Separations of Thirteen Phenolic Compounds using Single Peak Responses and an Interactive Computer Technique

Carlos Alberto P. Câmara, João Bortoloti, Ieda S. Scarminio, Cristiano A. Ballus, Adriana D. Meinhardt, Helena T. Godoy and Roy E. Bruns

Graphical Abstract

Experimental design-computer interactive simulation of an electropherogram is developed. The colored lines are calculated using response surface models. The corresponding experimental electropherogram is below

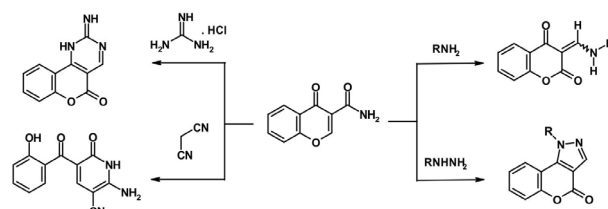


1754 Ring Transformation of Chromone-3-Carboxamide under Nucleophilic Conditions



Magdy A. Ibrahim

SI online

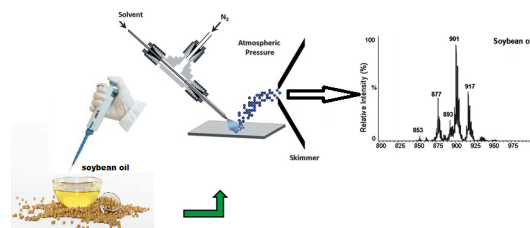


Graphical Abstract

A variety of heterocyclic systems was obtained from ring transformation of chromone-3-carboxamide under nucleophilic conditions

1764 Efficiencies of Acid and Base-Catalyzed Methylation of Vegetable Oils by Ambient Mass Spectrometry

Oscar O. Santos Júnior, Paula F. Montanher, Elton G. Bonafé, Swami A. Maruyama, Fabiana Carbonera, Rosana M. Alberici, Marcos N. Eberlin and Jesuí V. Visentainer



Graphical Abstract

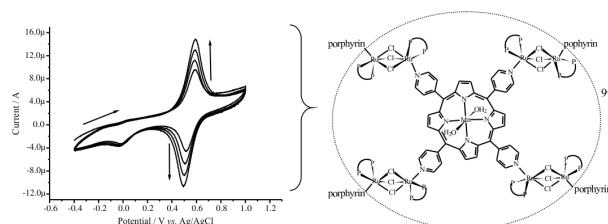
This work aimed at comparing the performance of acid and base-catalyzed soybean oil methylation methods used for FA analysis. For this comparison, gas chromatography (GC) and easy ambient sonic spray ionization (EASI-MS) were used for chemical monitoring

1772 Electropolymerized Supramolecular Tetraruthenated Porphyrins Applied as a Voltammetric Sensor



Monize M. da Silva, Gabriel H. Ribeiro, Alzir A. Batista, Anizio M. de Faria, André L. Bogado and Luis R. Dinelli

SI online



Graphical Abstract

The supramolecular tetraruthenated porphyrins, $\{Mn-TPyP(H_2O)_2[RuCl_3(dppb)]_4\}PF_6$, was immobilized on a glassy carbon electrode by electropolymerization and used as a sensor for acetaminophen

1781 QSAR Models of Reaction Rate Constants of Alkenes with Ozone and Hydroxyl Radical

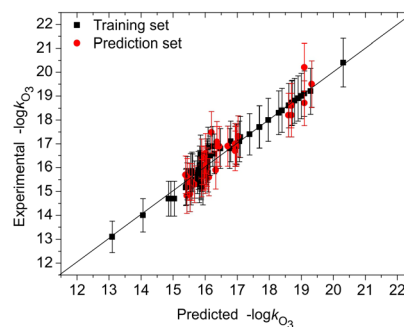


Yueyu Xu, Xinliang Yu and Shihua Zhang

SI online

Graphical Abstract

Quantum chemical descriptors for QSAR models of reaction rate constants k_{O_3} and k_{OH} of alkenes with ozone and OH radical were obtained from ground-state and transition-state structures of degradation processes. The present work tests that transition states have important effects on k_{O_3} and k_{OH} of degradation processes. Our models overcome the defect of literature models that only used the ground-state descriptors to build QSAR models for k_{O_3} and k_{OH}

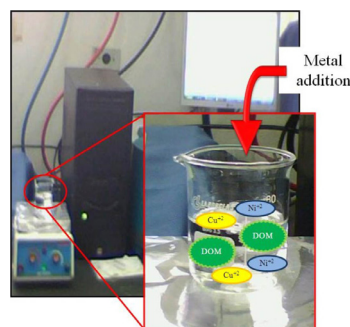


1789 Copper(II) and Nickel (II) Complexation Capacity of Dissolved Organic Matter from Rivers of Agricultural and Urban Areas in the State of São Paulo

Amanda M. Tadini, Mariele B. Campanha, Altair B. Moreira and Márcia C. Bisinoti

Graphical Abstract

In the present work was evaluated the complexation capacity and conditional stability constant of organic matter from typical agricultural areas and from urban areas with copper and nickel ions was evaluated using a luminescence spectrofluorometer



1798 Molecular Modeling and Anticholinesterasic Activity of Novel 2-Arylamino-cyclohexyl N,N-Dimethylcarbamates

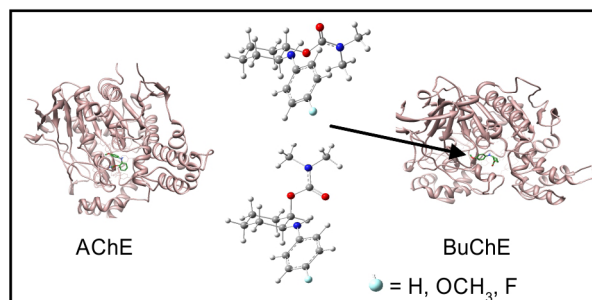


Mariane C. Bagatin, Augusto A. Cândido, Glaucia M. S. Pinheiro, Nelci F. Höehr, Miguel Machinski Jr., Simone A. G. Mossini, Ernani A. Basso and Gisele F. Gauze

SI online

Graphical Abstract

The novel synthesized carbamates are selective inhibitors of the BuChE enzyme. According to molecular docking calculations, the carbamoyl group is close to the key residues of the catalytic triad

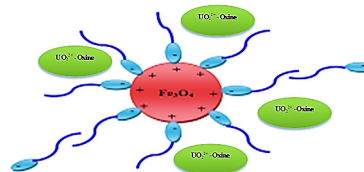


1808 Spectrophotometric Determination of Trace Amounts of Uranium(VI) using Modified Magnetic Iron Oxide Nanoparticles in Environmental and Biological Samples

Gholamreza Khayatani, Shahed Hassanpoor, Amir R. J. Azar and Sajjad Mohebbi

Graphical Abstract

A Fe_3O_4 magnetic nanoparticle modified by sodium dodecyl sulfate was synthesized for preconcentration and determination of uranium(VI) as an uranium(VI)-oxine complex. The method shows appropriate detectability, linearity, precision and accuracy and can be applied for the analyses of natural waters, granite rocks, urine and blood serum samples



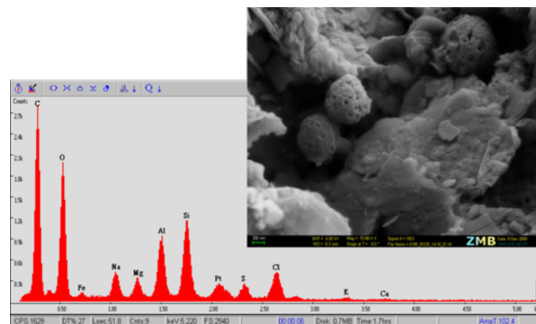
1818 Reconstructing Historical Changes in Combustion Patterns by Means of Black Carbon and PAH Evaluation in Dated Sediments from Guanabara Bay, Rio de Janeiro

SI online

Cristiane R. Mauad, Angela de L. R. Wagener, Cássia de O. Farias, Naira M. S. Ruiz, Renato S. Carreira, Crisógono Vasconcelos, José M. Godoy, Sonia M. C. de Menezes, Arthur de L. Scofield

Graphical Abstract

The figure shows the micrograph of black carbon spheres and its elementary composition in sediment sample of Guanabara Bay by SEM/EDX

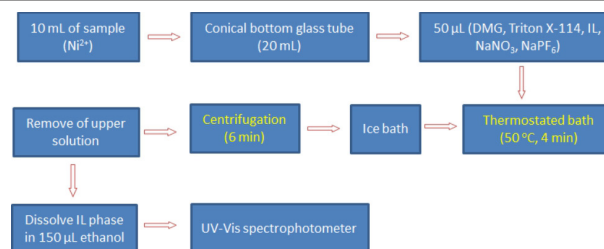


1832 Cold-Induced Aggregation Microextraction Technique based on Ionic Liquid for Preconcentration and Determination of Nickel in Food Samples

Bahram Ebrahimi, Soleiman Bahar and Seyde Elham Moedi

Graphical Abstract

This scheme shows the proposed method for the determination of nickel after preconcentration using cold-induced aggregation microextraction (CIAME)



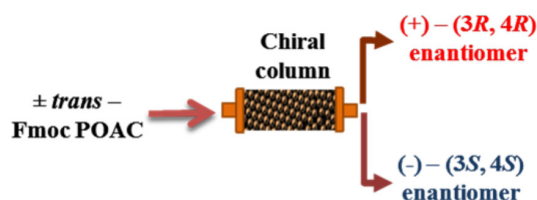
1840 Alternative and Simple Normal-Phase HPLC Enantioseparation of a Chiral Amino Acid-Type Spin Label Derivative

SI online

Joao P. F. Vieira, Erick F. Poletti, Renata F. F. Vieira, Vinicius Veredas, Cesar C. Santana and Clovis R. Nakaie

Graphical Abstract

Enantioseparation of *trans*-Fmoc-POAC spin label

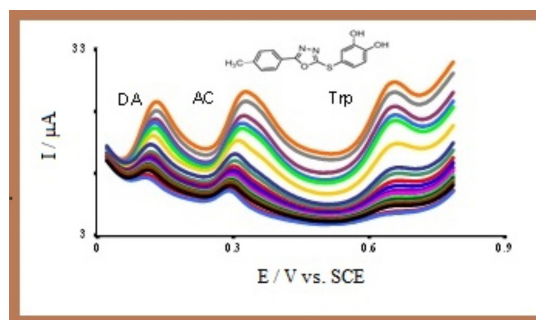


1846 Developing a Sensor for the Simultaneous Determination of Dopamine, Acetaminophen and Tryptophan in Pharmaceutical Samples Using a Multi-Walled Carbon Nanotube and Oxadiazole Modified Glassy Carbon Electrode

Navid Nasirizadeh, Zahra Shekari, Hamid R. Zare, Seied A. Y. Ardakani and Hamid Ahmar

Graphical Abstract

Oxadiazole derivative on multi-walled carbon nanotubes glassy carbon electrode was constructed by electrodeposition of oxadiazole on a MWCNT modified GCE. OMWCNT-GCE exhibits excellent electrocatalytic activity for dopamine oxidation. This modified electrode resolved the overlapping of the anodic peaks DA, AC and Trp

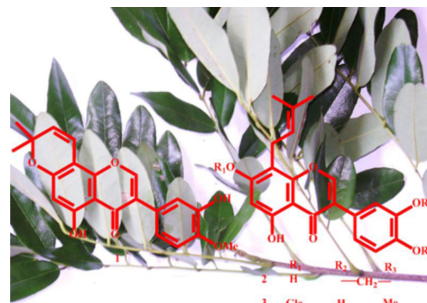


1857 New Isoflavones from the Leaves of *Vatairea guianensis* Aublé

Ronilson Freitas de Souza, Victor H. S. Marinho,
Geilson A. da Silva, Livio M. Costa-Jr., Joyce Kelly R. da Silva,
Gilmar N. T. Bastos, Alberto C. Arruda, Milton N. da Silva
and Mara Silvia P. Arruda



SI online


Graphical Abstract

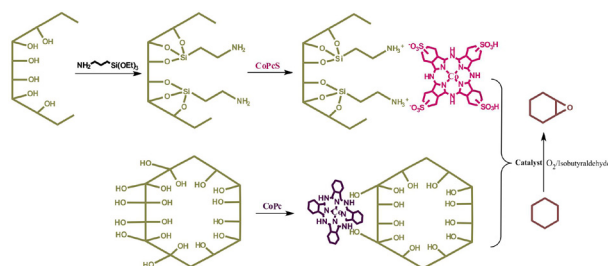
Isoflavones 1-3 are new natural products isolated from the leaves of *Vatairea guianensis* Aublé. The ethanol extract from the leaves and the isolated compounds (1-3) were evaluated for their potential scavenging DPPH[•].

1864 Immobilization of Cobalt Phthalocyanine and Tetrasulfophthalocyanine onto MCM-41 and MCM-48: Effect of Immobilization Method on Catalytic Activity

Mahtab Pirouzmand, Mostafa M. Amini, Nasser Safari and
Touba Hamoule



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Graphical Abstract

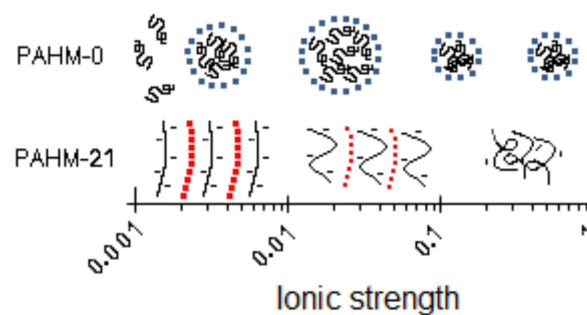
Cobalt tetrasulfophthalocyanine was anchored onto the surface of NH₂-MCM-41 and NH₂-MCM-48. Physical mixtures of CoPc in MCM-41 and in MCM-48 were also prepared. The catalytic properties of these materials were studied in the aerobic epoxidation of cyclohexene.

1871 Polyelectrolyte and Non-Polyelectrolyte Polyacrylamide Copolymer Solutions: the Role of Salt on the Intra- and Intermolecular Interactions

Ana M. S. Maia, Marcos A. Villetti, Redouane Borsali and
Rosângela C. Balaban



SI online


Graphical Abstract

This work supports the existence of a slow relaxation mode in polymer solutions due to diffusion and the internal motions of these transient clusters for poly(acrylamide-co-dihexylacrylamide) (PAHM-0) and poly(acrylamide-co-sodium acrylate-co-dihexylacrylamide) (PAHM-21) to the self-diffusion of individual chains retarded by interchain friction.

1880 Assessment of Direct Mercury Analyzer® to Quantify Mercury in Soils and Leaf Samples

Jose J. Melendez-Perez and Anne H. Fostier


Graphical Abstract

A method for mercury quantification in leaves and soil samples by direct sample combustion analysis was assessed and validated.