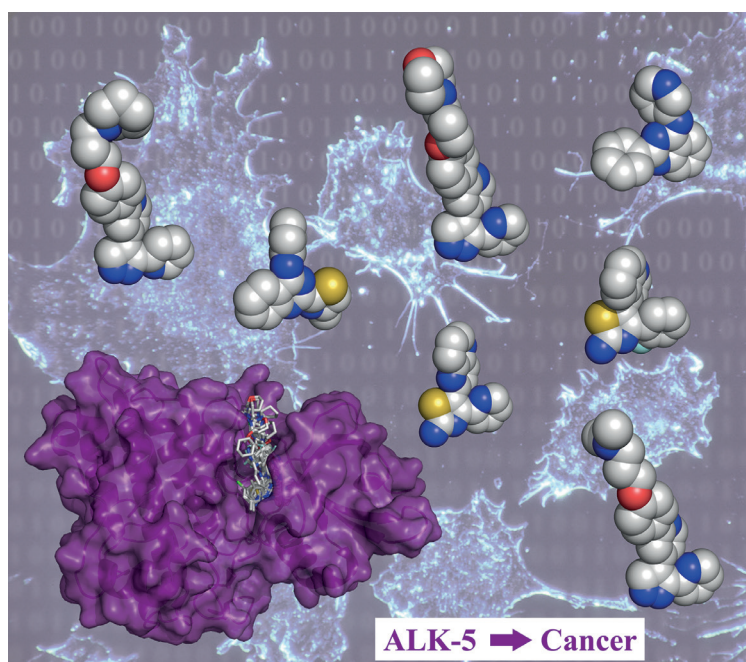


Cover Picture



Activin-like kinase 5 (ALK-5) receptor is considered a key target for the cancer treatment and there are several classes of ALK-5 inhibitors reported in the literature. Quantitative structure-activity relationship (QSAR) models are important to describe the main physicochemical properties related to the biological activity of bioactive ligands. From a set of ALK-5 inhibitors and electronic, molecular, stereochemical and topological descriptors, different techniques of variable selection in combination with partial least squares regression were employed to construct reliable multivariate models. Details are presented in the Article **ALK-5 Inhibition: A Molecular Interpretation of the Main Physicochemical Properties Related to Bioactive Ligands** by Sheila C. Araujo, Vinicius G. Maltarollo, Danielle C. Silva, Jadson C. Gertrudes and Kathia M. Honorio on page 1936.

Contents

Editorial

1743 **Thought for Food**
Fernando Galembeck

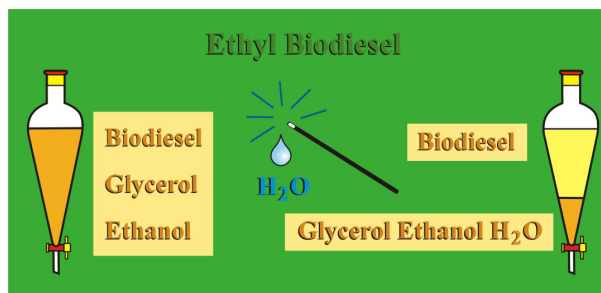
Articles

1745 Separation of the Glycerol-Biodiesel Phases in an Ethyl Transesterification Synthetic Route Using Water

Willian L. G. da Silva, Patrícia T. de Souza, Gustavo G. Shimamoto and Matthieu Tubino

Graphical Abstract

In the synthesis of an ethyl biodiesel prepared through a transesterification reaction, the separation of the glycerol from the biodiesel phase is facilitated by the addition of water



1751 New and Sensitive Electroquantification of Sulfentrazone in Soil by Differential-Pulse Voltammetry

Mariana N. Catrinck, Leonardo L. Okumura, Antonio A. Silva, Adelir A. Saczk and Marcelo F. Oliveira

Graphical Abstract

Sulfentrazone was analyzed directly in the soil sample without any cleaning step or pre-concentration by differential-pulse voltammetry



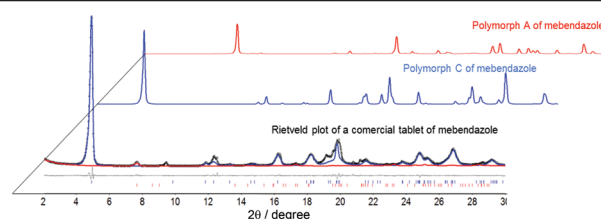
1760 Rietveld Method in the Analysis of Polymorphism in Mebendazole Tablets Acquired in Brazil's Drugstores

Simone T. B. Salvi, Selma G. Antonio, Fabio F. Ferreira and

Carlos O. Paiva-Santos



SI online



Graphical Abstract

Using X-ray powder diffraction and the Rietveld method to identify mebendazole polymorphs in solid formulations as well as to quantify mebendazole polymorphs in solid formulations available in Brazilian market

1769 Layered Zinc Hydroxide Salts Intercalated with Anionic Surfactants and Adsorbed with UV Absorbing Organic Molecules

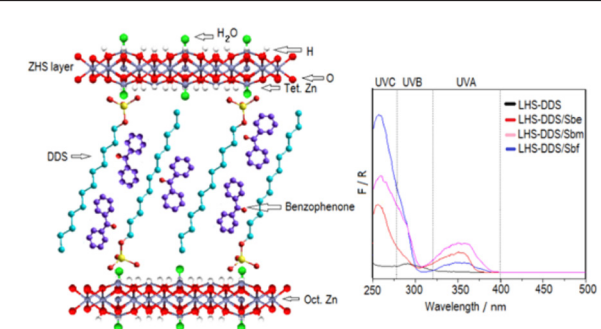


SI online

Ana C. T. Cursino, Vicente Rives, Luís D. Carlos, João Rocha and Fernando Wypych

Graphical Abstract

Layered zinc hydroxides intercalated with two surfactants were adsorbed with different neutral UV absorbing molecules. The materials have potential to be used in new sunscreens formulations



1781 Solubility and Bioaccessibility of Ba, Ca, Cr, Cu, Fe, Mg, Mn, P, Sr and Zn in Slim Coffee Infusions by *in vitro* Gastrointestinal Digestion

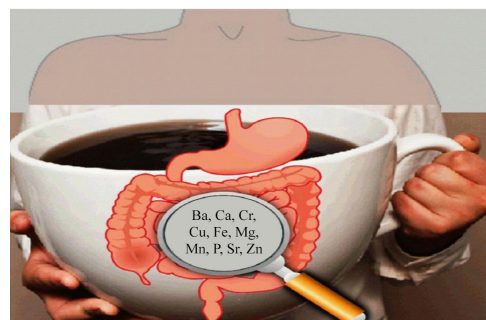


SI online

Anna Szymczycha-Madeja, Maja Welna and Pawel Pohl

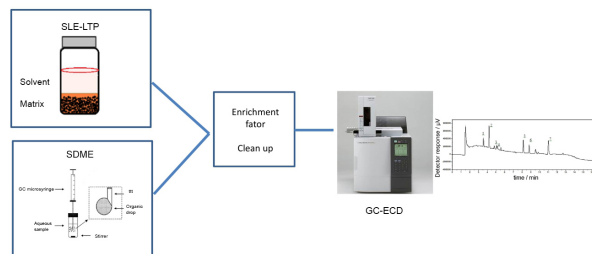
Graphical Abstract

The solubility and the bioaccessibility of macro- (Ca, Mg, P), essential trace (Cu, Fe, Mn, Zn) and non-essential trace (Ba, Cr, Sr) elements of the slim coffee products were evaluated by the *in vitro* gastrointestinal digestion



1790 Determination of Pesticides in Soil Using a Hyphenated Extraction Technique

Carlos E. S. Soares, Antônio A. Neves, Maria E. L. R. Queiroz,
André F. Oliveira, Anna I. G. Costa, Roberta C. Assis and
Carlos Eduardo O. Andrade

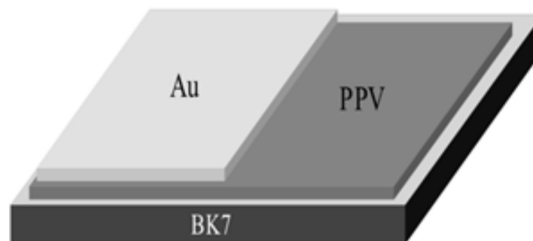


Graphical Abstract

Application of single drop microextraction in solid samples. This method consists of hyphenation techniques already existing: solid-liquid extraction with low temperature partitioning and single drop microextraction

1798 Effects from Gold Electrodes on the Electron-Phonon Coupling of Poly(*p*-phenylenevinylene) Films

Eralci M. Therézio, Ángel A. Hidalgo, Osvaldo N. Oliveira Jr.,
Raígn A. Silva and Alexandre Marletta



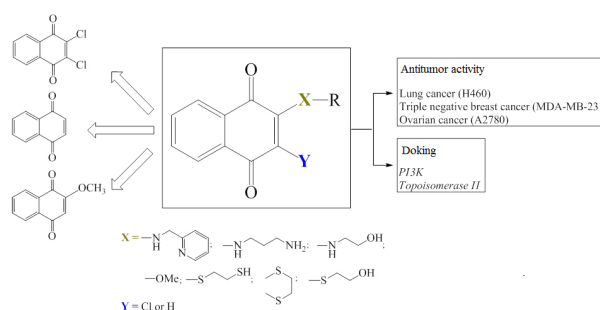
Graphical Abstract

Au clusters interaction occurs with the phenyl rings. These results predict effects from metallic electrodes deposited on polymer films. The results are consistent with theoretical predictions in *ab initio* calculations

1804 Synthesis, Antitumor Activity and Docking of 2,3-(Substituted)-1,4-Naphthoquinone Derivatives Containing Nitrogen, Oxygen and Sulfur

SI online

Maicon Delarmelina, Renata D. Daltoé, Murilo F. Cerri,
Klesia P. Madeira, Leticia B. A. Rangel, Valdemar Lacerda
Júnior, Wanderson Romão, Alex G. Taranto and
Sandro J. Greco

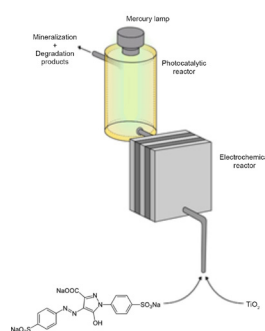


Graphical Abstract

Eleven 1,4-naphthoquinone derivatives were synthesized, their cytotoxic effects on cancer cells were evaluated and docking studies were conducted

1817 Dye Degradation Enhanced by Coupling Electrochemical Process and Heterogeneous Photocatalysis

Lidiaíne M. Santos, Kamila P. de Amorim, Leonardo S.
Andrade, Paulo S. Batista, Alan G. Trovó and Antonio E. H.
Machado



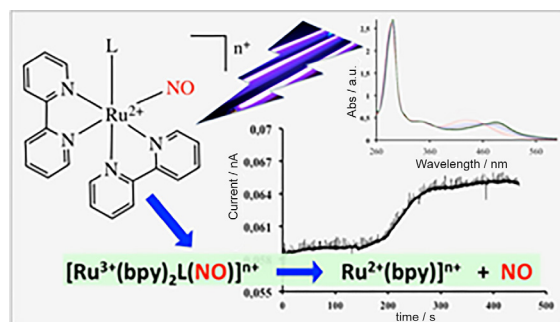
Graphical Abstract

The combination between an electrochemical process and heterogeneous photocatalysis for dye degradation resulted in 74% of mineralization in 120 min of reaction, a value 30% higher than the sum of the results obtained by heterogeneous photocatalysis (44%) and electrochemical oxidation (13%)

1824 Photochemical and Electrochemical Study of the Release of Nitric Oxide from $[\text{Ru}(\text{bpy})_2\text{L}(\text{NO})](\text{PF}_6)_n$ Complexes ($\text{L} = \text{Imidazole, 1-Methylimidazole, Sulfite and Thiourea}$), Toward the Development of Therapeutic Photodynamic Agents

SI online

Manuela C. L. Cândido, Arquimedes M. Oliveira, Francisco
O. N. Silva, Alda K. M. Holanda, Walysson Gomes Pereira,
Eduardo H. S. Sousa, Zumira A. Carneiro, Roberto S. Silva and
Luiz G. F. Lopes



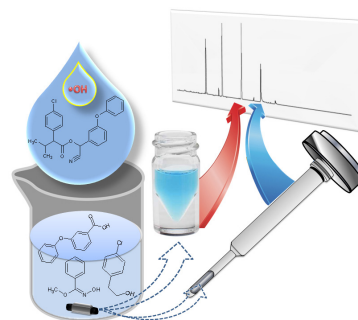
Graphical Abstract

The photochemical release of nitric oxide from complex type $[\text{Ru}(\text{bpy})_2\text{LX}]^{n+}$ was investigated. The amount of NO released from the complexes upon irradiation was determined using a new developed method through square wave voltammetry

- 1831 Screening of By-Products of Esfenvalerate in Aqueous Medium Using SBSE Probe Desorption GC-IT-MS Technique**
 Renata Colombo, Tanare C. R. Ferreira, Janete H. Yariwake and Marcos R. V. Lanza

Graphical Abstract

Esfenvalerate degradation products were obtained by chemical oxidation with hydrogen peroxide and analyzed by stir bar sorptive extraction (SBSE) liquid and thermal desorption. Their structure was elucidated using SBSE technique and probe desorption gas chromatography-ion trap mass spectrometry (GC-IT-MS) analysis



- 1838 Ruthenium(II) Complexes Containing Anti-Inflammatory Drugs as Ligands: Synthesis, Characterization and *in vitro* Cytotoxicity Activities on Cancer Cell Lines**

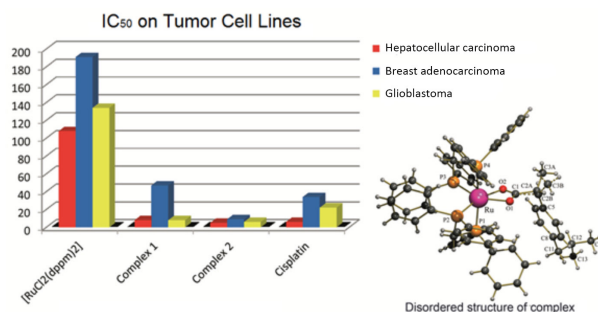


SI online

Junai C. S. Lopes, Jaqueline L. Damasceno, Pollyanna F. Oliveira, Adriana P. M. Guedes, Denise C. Tavares, Victor M. Deflon, Norberto P. Lopes, Marcos Pivatto, Alzir A. Batista, Pedro I. S. Maia and Gustavo Von Poelhsitz

Graphical Abstract

Two new ruthenium(II) complexes containing diclofenac and ibuprofen anions as coligands were active against human tumor cell lines

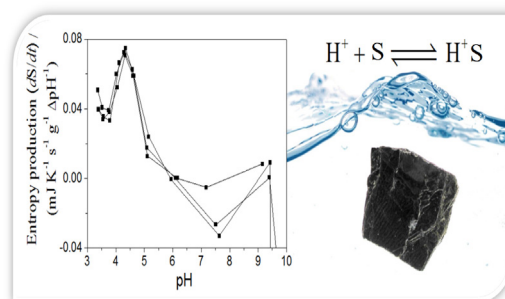


- 1848 Potentiometric Titration and Out-Of-Equilibrium pH Response of the Biotite-Water System**

Vicente R. Almeida, Bruno Szpoganicz and Steeve Bonneville

Graphical Abstract

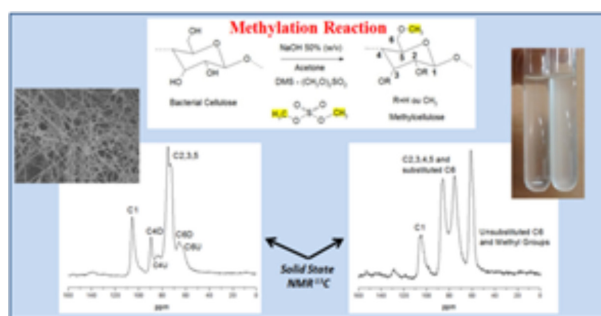
“Slow” proton exchange entropy production in the biotite-water complex system (S) shows that biotite offers acidification-resistant relations to soils and natural environment



- 1861 Synthesis and Characterization of Methylcellulose Produced from Bacterial Cellulose under Heterogeneous Condition**
 Rafael L. Oliveira, Júlia G. Vieira, Hernane S. Barud, Rosana M. N. Assunção, Guimes R. Filho, Sidney J. L. Ribeiro and Younes Messadeq

Graphical Abstract

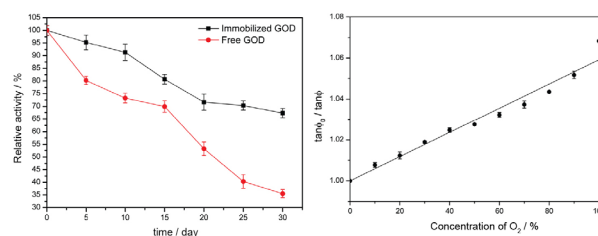
Methylcellulose (MC) was produced from bacterial cellulose, using dimethyl sulfate under heterogeneous conditions. A material with a high degree of substitution (DS) was obtained



- 1871 Bifunctional Porous SiO₂ Complex Nanoparticles with Properties of Enzymatic Catalysis and Optical Oxygen Sensing**
 Jun Huang, Kun Li, Huichao Liu and Liyun Ding

Graphical Abstract

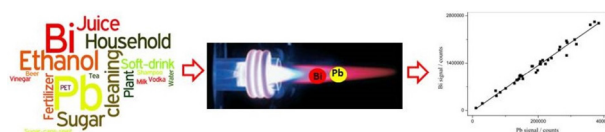
The complex particles have improved enzyme stability of storage compared with free glucose oxidase (GOD) and optical oxygen sensing property



1879 Contributions on the Use of Bismuth as Internal Standard for Lead Determinations Using ICP-Based Techniques

Marcos A. Bechlin, Edilene C. Ferreira, José A. Gomes Neto, Juliano C. Ramos and Daniel L. G. Borges

SI online



Graphical Abstract

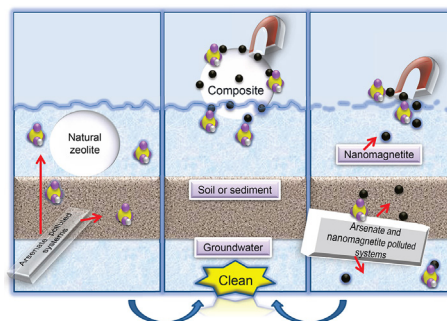
Bismuth was evaluated as a general internal standard in lead determinations in inductively coupled plasma-based techniques in a great variety of sample matrices

1887 Nanomagnetite-Zeolite Composites in the Removal of Arsenate from Aqueous Systems

Carmen Pizarro, María A. Rubio, Mauricio Escudey, María F. Albornoz, Daniela Muñoz, Juliano Denardin and José D. Fabris

Graphical Abstract

Supported nanomagnetite reduces the difficulty of separating nanoparticles from aqueous suspensions, where the use of unsupported nanoparticles is likely to lead to eventual contamination of soils, sediments, runningwater and groundwater sources

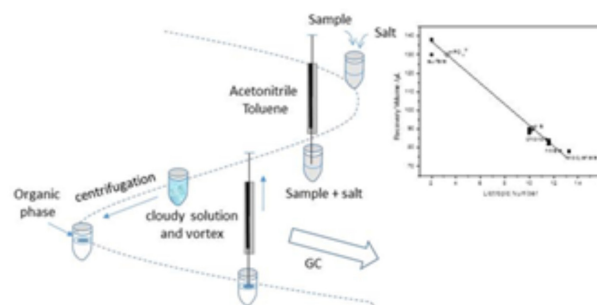


1897 Evaluation of the Effects of Hofmeister Series on Salting Out in the Determination of Organophosphorous Pesticides and Pyrethroids by LDS/DLLME

Luiz M. S. Noronha, Antonio A. Neves, Maria E. L. R. Queiroz and André F. Oliveira

Graphical Abstract

The influence of Voet lyotropic number of salts in aqueous phase on volume of organic phase in dispersive liquid-liquid microextraction (DLLME) for pesticides determination



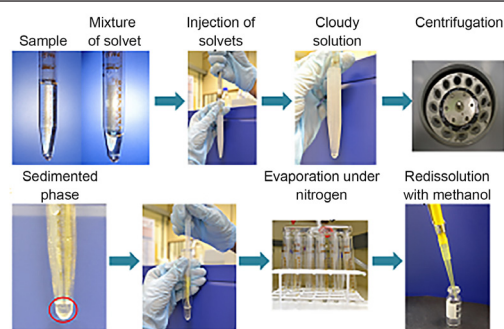
1902 Dispersive Liquid-Liquid Microextraction with Liquid Chromatography-Tandem Mass Spectrometry for the Determination of Triazine, Neonicotinoid, Triazole and Imidazolinone Pesticides in Mineral Water Samples

SI online

Cátia M. Bolzan, Sergiane S. Caldas, Bruno S. Guimarães and Ednei G. Primei

Graphical Abstract

Dispersive liquid-liquid microextraction (DLLME) was successfully used for the extraction of neonicotinoid, triazole and imidazolinone pesticides in mineral water samples



1914 *p*-Cymenesulphonyl Chloride: A Bio-Based Activating Group and Protecting Group for Greener Organic Synthesis

Thomas J. Farmer, James H. Clark, Maite L. Gothe, Duncan J. Macquarrie and James Sherwood

SI online

Graphical Abstract

p-Cymenesulphonyl chloride can be synthesised from abundant sources of citrus waste for use in organic chemistry as a protecting and activating group

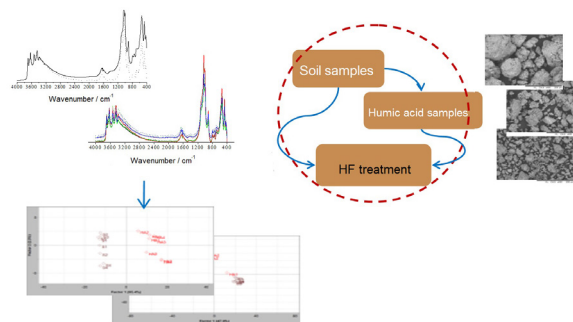


1920 Instrumental and Experimental Conditions for the Application of Fourier Transform Infrared Analysis on Soil and Humic Acid Samples, Combined with Chemometrics Tools and Scanning Electron Microscopy

Nathalie Merlin, Vanderlei A. Lima, Larissa M. Santos-Tonial

Graphical Abstract

Study about soil and humic acid samples by Fourier transform infrared spectroscopy (instrumental conditions of background and baseline), supported by the use of chemometric tools. Samples were also studied by scanning electron microscopy

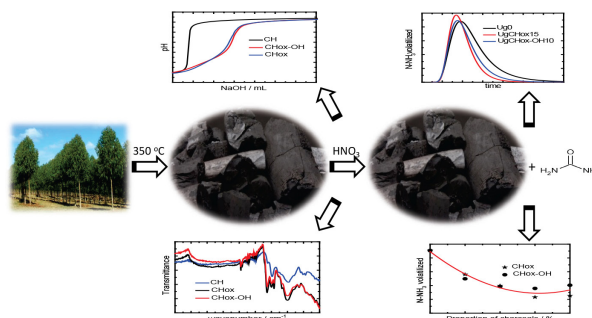


1928 Volatilization of Ammonia Originating from Urea Treated with Oxidized Charcoal

Geilton G. F. Guimarães, Diogo M. Paiva, Reinaldo B. Cantarutti, Edson M. Mattiello and Efraim L. Reis

Graphical Abstract

Charcoal of eucalyptus tree was obtained by heating at 350 °C and after was oxidized with HNO₃. The charcoal was characterized by acid-base potentiometric titration and infrared spectroscopy. The charcoal was mixed with urea and the volatilization of NH₃ was evaluated in the time and with various charcoal proportions



1936 ALK-5 Inhibition: A Molecular Interpretation of the Main Physicochemical Properties Related to Bioactive Ligands

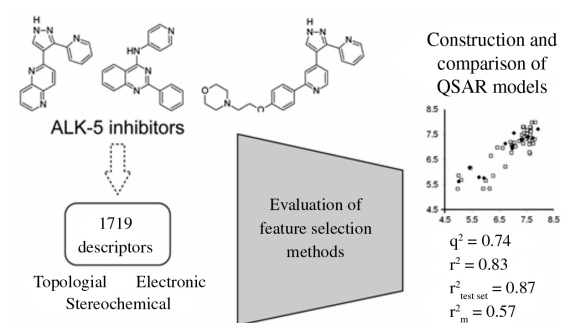
Sheila C. Araujo, Vinicius G. Maltarollo, Danielle C. Silva, Jadson C. Gertrudes and Kathia M. Honório



SI online

Graphical Abstract

Studies of quantitative structure-activity relationships were performed to explore the relationship between the molecular structure of 1,5-naphthyridine, pyrazole and quinazoline derivatives and the inhibition of the activin-like kinase 5, a biological target related to the cancer treatment

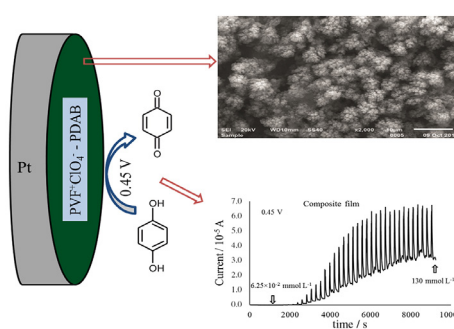


1947 Synthesis of Poly(Vinylferrocene) Perchlorate/Poly(3,3'-Diaminobenzidine) Modified Electrode in Dichloromethane for Electroanalysis of Hydroquinone

Emine Ülker and Muammer Kavanoz

Graphical Abstract

PVF⁺ClO₄⁻-PDAB composite film was potentiodynamically synthesized for the first time on Pt disc electrode. Prepared film had porous structure. The film was used for amperometric determination of hydroquinone and it was found sensitive to hydroquinone. Lower limit of detection and broad linear range were obtained



1956 Coupling DLLME-CE for the Stereoselective Analysis of Venlafaxine and Its Main Metabolites after Biotransformation by Fungi

Marcela A. Bortoletto, Mariana Z. Bocato, Mônica T. Pupo, Cristiane M. Gaitani and Anderson R. M. Oliveira

Graphical Abstract

Stereoselective biotransformation of *rac*-venlafaxine into (+)-(*S*)-*N*-desmethylvenlafaxine by the fungus *Cunninghamella elegans* ATCC 10028B with an enantiomeric excess of 100%

