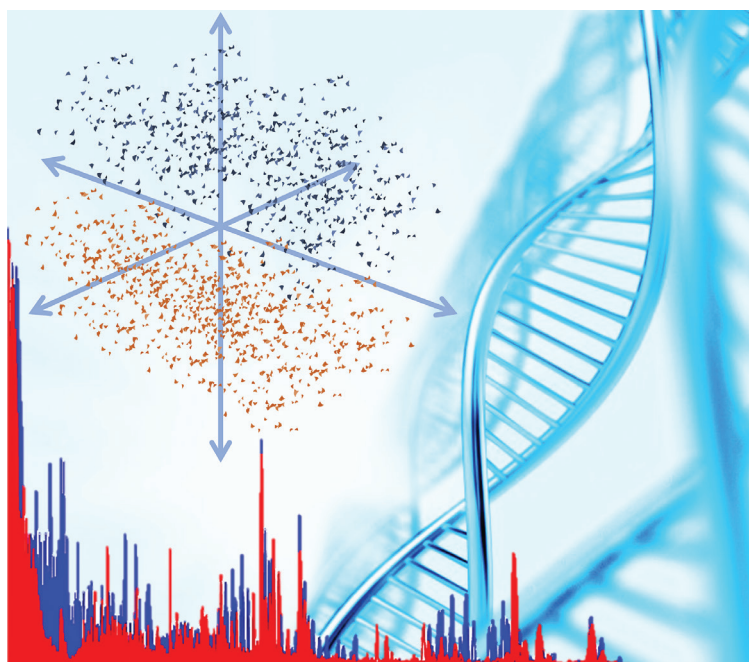


Cover Picture



This paper reports the use of chemometric techniques employed for discrimination of cancer samples based on mass spectra data sets. The artwork shows a representative mass spectrum with colors referring to two different classes and a scatter plot showing its discrimination in a three-dimensional aspect. In the background, a DNA molecule due to its importance for cancer differentiation. Details are presented in the Article **Principal Component Analysis with Linear and Quadratic Discriminant Analysis for Identification of Cancer Samples Based on Mass Spectrometry** by *Camilo L. M. Morais and Kássio M. G. Lima* on page 472.

Contents

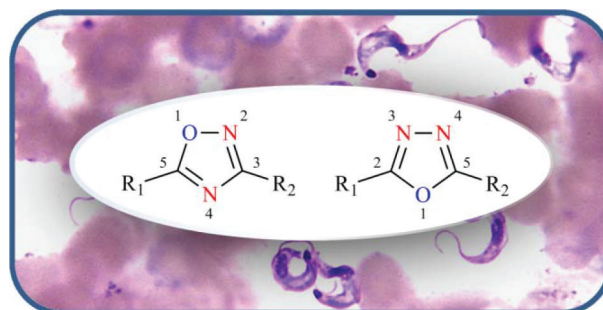
Review

435 1,2,4- and 1,3,4-Oxadiazoles as Scaffolds in the Development of Antiparasitic Agents

Paulo Pitasse-Santos, Vitor Sueth-Santiago and Marco E. F. Lima

Graphical Abstract

This review focuses on the importance of 1,2,4- and 1,3,4-oxadiazole cores in the design of new antiparasitic drugs. Here are highlighted the synthetic methodologies for their preparation as well as physicochemical differences between the isomers and their binding properties with biological receptors.



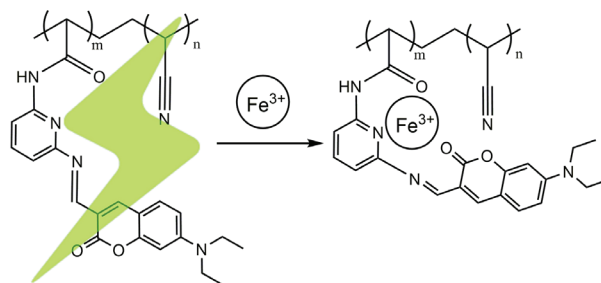
Articles

457 A Novel Nanofibrous Film Chemosensor for Detecting and Adsorbing Fe^{3+}



Chen Zhou, Yinan Zhang and Heng Liu

SI online



Graphical Abstract

Recognition of the nanofibrous film chemosensor for Fe^{3+} by decrease of fluorescence.

463 Effects of a Diet Supplemented with Japanese Grape (*Hovenia dulcis*) Seed Oil on the Omega-3 and Nutritional Lipid Quality in Nile Tilapia (*Oreochromis niloticus*)

Marina Oliveira, Ricardo P. Ribeiro, Michele C. da Silva, Paula F. Montanher, Fabiana Carbonera, Jesuí V. Visentainer and Liane Maldaner



Graphical Abstract

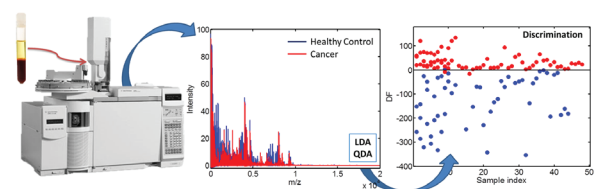
Japanese grape seed oil (JGSO) is rich in alpha-linolenic acid (LNA) and was used to prepare supplemented diets for Nile tilapia. The replacement of soybean oil with JGSO in the prepared diets raises the nutritional lipid quality of the freshwater fish.

472 Principal Component Analysis with Linear and Quadratic Discriminant Analysis for Identification of Cancer Samples Based on Mass Spectrometry



Camilo L. M. Morais and Kássio M. G. Lima

SI online



Graphical Abstract

Principal component analysis with linear discriminant analysis (PCA-LDA) and quadratic discriminant analysis (PCA-QDA) were applied for discrimination between healthy control and cancer samples (ovarian and prostate cancer) based on mass spectra data sets.

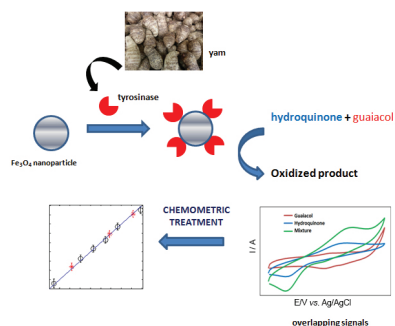
482 Simultaneous Determination of Different Phenolic Compounds Using Electrochemical Biosensor and Multivariate Calibration



Renata K. Mendes, Marcos V. C. Dantas, Alessandra B.

SI online

Nogueira, Augusto Etcheagaray, Paulo R. Filgueiras and Ronei J. Poppi



Graphical Abstract

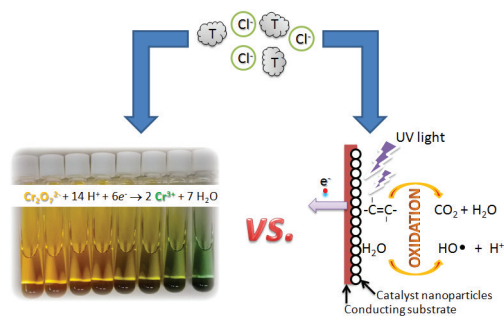
A biosensor based on tyrosinase immobilized onto iron magnetic nanoparticles was successfully used for the simultaneous determination of two phenolic compounds after data analysis and chemometric treatment.

490 The Dichromate Method versus the Photoelectrochemical Method: the Synergistic Influence of Turbidity and Chlorides on Chemical Oxygen Demand Analysis

Gabriel O. Quintana, Enelton Fagnani, Fernando P. Candello and José R. Guimarães

Graphical Abstract

The combined effect of turbidity and chlorides on chemical oxygen demand have not been explored before this study and must be considered when the acid dichromate method is replaced by photoelectrochemical method.



499 Fine and Coarse Aerosol at Rio de Janeiro prior to the Olympic Games: Chemical Composition and Source Apportionment



Maria Luíza D. P. Godoy, Ana C. Almeida, Gisele B. Tonietto and José Marcus Godoy

SI online

Graphical Abstract

Aerosol sampler installed at Tijuca sampling station, showing both EPA design PM₁₀ inlets, one for elemental analysis (left) and the other for carbon determination (right).



509 Antimicrobial Diterpene from the Brazilian Termite *Nasutitermes macrocephalus* (Isoptera: Termitidae: Natutitermitinae)

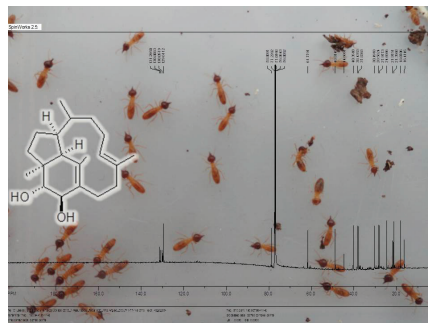


Márcia N. S. de la Cruz, Helvécio M. dos Santos Júnior, Denilson F. Oliveira and Claudia M. Rezende

SI online

Graphical Abstract

A new trinervitane diterpene isolated from termite soldiers (*Nasutitermes macrocephalus*) presented antimicrobial activities against *S. aureus* and *C. albicans*.



515 An *in silico* Study of Benzophenone Derivatives as Potential Non-Competitive Inhibitors of *Trypanosoma cruzi* and *Leishmania Amazonensis* Cysteine Proteinases

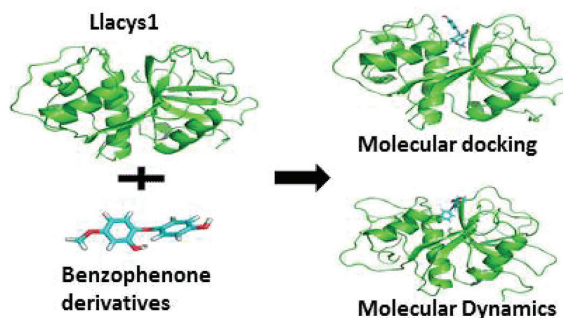


Poliany G. Freitas, Thiago E. Castilho, Leticia de Almeida, Claudia M. Maciel-Rezende, Luciano T. Costa, Claudio Viegas Junior, Marcos J. Marques, Marcelo H. dos Santos and Nelson J. F. da Silva

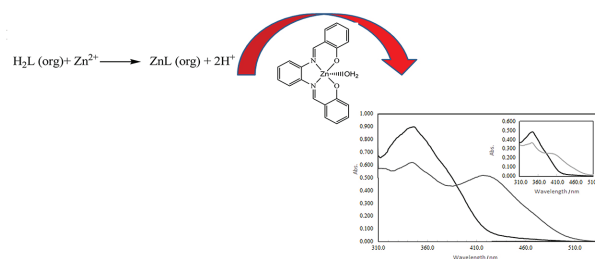
SI online

Graphical Abstract

The mechanism of interaction between benzophenone derivatives and cruzain and Llacys1 (the protein expressed by cysteine protease gene isoform 1 of *L. amazonensis*) by homology modelling, docking and molecular dynamics simulation.



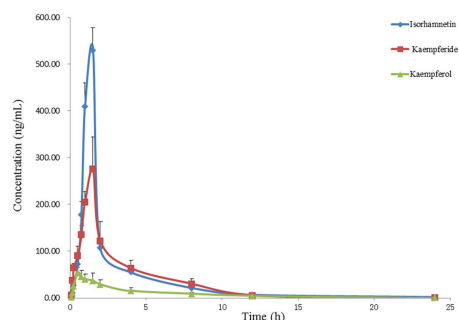
- 528** A Novel Sensitive Bulk Optode Based on 5-Br Salophen as an Ionophore for Determination of Zinc Ion in Real Samples
 Elham Alian, Abolfazl Semnani, Alireza Firooz and Mahboube Shirani



Graphical Abstract

The decrease of the concentration of 5-Br salophen in presence of Zn^{2+} in organic phase leads to an optical sensor, in which the mechanism is described by ion-exchange.

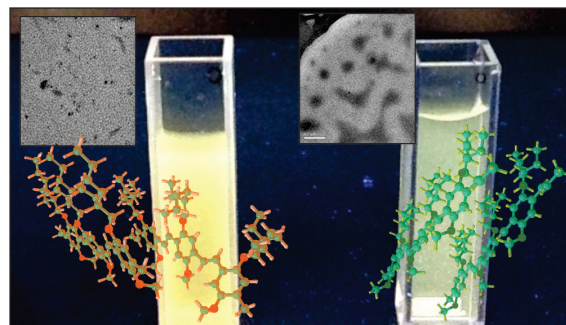
- 535** Simultaneous Determination of Kaempferide, Kaempferol and Isorhamnetin in Rat Plasma by Ultra-High Performance Liquid Chromatography-Tandem Mass Spectrometry and its Application to a Pharmacokinetic Study
 Zhitao Jiang, Jianchun Wang, Xiaofeng Chen, Xue Wang, Tongfang Wang, Zhitao Zhu and Jinhua Pan



Graphical Abstract

The mean plasma concentration-time curves after an oral administration of *Sedum sarmentosum* Bunge extract are shown. The data conformed to a two-compartment, first-order pharmacokinetic model.

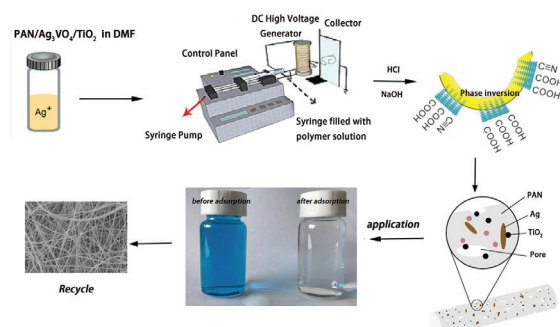
- 543** Photoluminescence of Solvent-Selected Fluorescent Moieties in MEH-PPV Solutions and Films
 Antonio C. C. Ribeiro, Henrique S. Camargo, Douglas H. Pereira, Rogério Custódio and Tatiana D. Martins



Graphical Abstract

The photophysical behavior of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) is morphology-dependent in both solution and film form: the preparation method influences the exciton distribution.

- 560** Development of a Novel Mixed Titanium, Silver Oxide Polyacrylonitrile Nanofiber as a Superior Adsorbent and its Application for MB Removal in Wastewater Treatment
 Zhiqun Xu, Congcong Wei, Jiali Jin, Wenkai Xu, Qiao Wu, Junjie Gu, Minrui Ou and Xiaoping Xu



Graphical Abstract

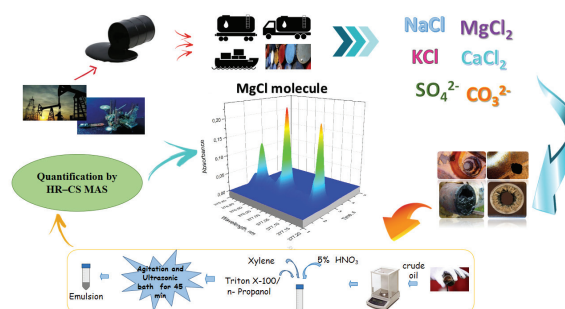
Development of a novel mixed titanium, silver oxide nanofiber as a superior adsorbent for dyes removal in the wastewater treatment.

571 Determination of Chlorine in Crude Oil Emulsified via the MgCl Molecule by HR-CS MAS

Izabel K. S. Oliveira, Rina L. S. Medeiros, Djalma R. Silva and Tatiane A. Maranhão

Graphical Abstract

Chlorine present in crude oil is an important cause of problems related to corrosion and damage to equipment. This paper describes the development of a method for chlorine determination in crude oil samples through MgCl diatomic molecule by high-resolution continuum source molecular absorption spectrometry (HR-CS MAS).

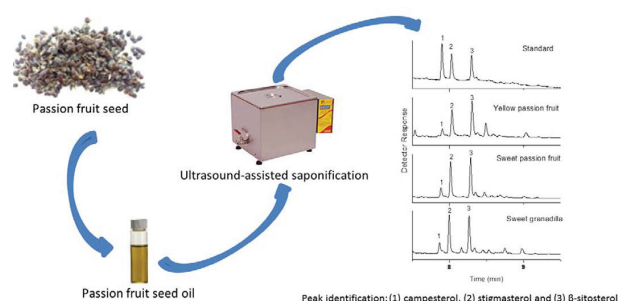


579 Ultrasound-Assisted Saponification Coupled with Gas Chromatography-Flame Ionization Detection for the Determination of Phytosterols from Passion Fruit Seed Oil

Eliza M. Rotta, Michele C. da Silva, Liane Maldaner and Jesuí V. Visentainer

Graphical Abstract

A method based on ultrasound-assisted saponification (UAS) was proposed to determine phytosterols in passion fruit seed oil. The optimized UAS method extracted higher phytosterol concentrations and was about 3.3 times faster than the conventional saponification method.

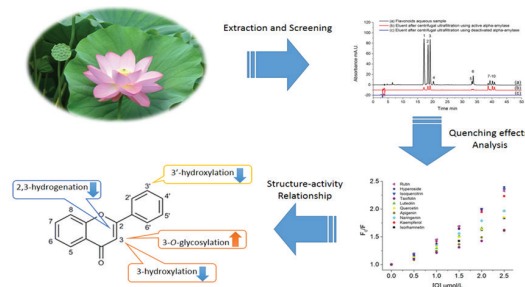


587 Screening and Binding Analysis of Flavonoids with Alpha-Amylase Inhibitory Activity from Lotus Leaf

Liping Liao, Jing Chen, Liangliang Liu and Aiping Xiao

Graphical Abstract

Centrifugal ultrafiltration combined with liquid chromatography was used to screen alpha-amylase inhibitors from ten flavonoids mixture and the binding degrees ranged from 2.34 to 94.1%.

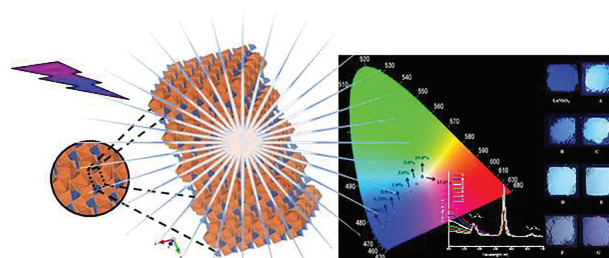


594 Effect of Dy³⁺ Amount on the Structural and Luminescence Properties of LaNbO₄:Dy³⁺ Phosphor Obtained by One-Step Spray Pyrolysis Process

Gabriela S. Freiria, Amanda L. Ribeiro, Marc Verelst, Eduardo J. Nassar and Lucas A. Rocha

Graphical Abstract

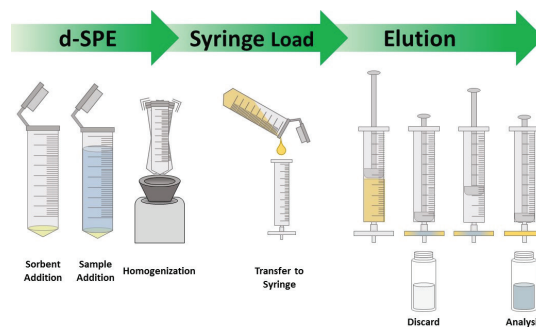
Blue-white tunable emission color in (Dy³⁺)-LaNbO₄ spherical particles synthesized by one-step spray pyrolysis process. The obtained CIE chromaticity coordinates fit the National Television Standard Committee (NTSC) standard values.



- 602** **Determination of Six Synthetic Dyes in Sports Drinks by Dispersive Solid-Phase Extraction and HPLC-UV-Vis**
 Luana Floriano, Lucila C. Ribeiro, Nathália Saibt,
 Nelson M. G. Bandeira, Osmar D. Prestes and Renato Zanella

Graphical Abstract

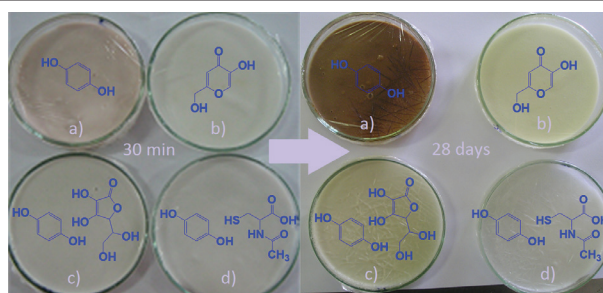
Simple and fast dispersive solid-phase extraction (d-SPE) method combined with syringe/filter to perform dyes analysis by high-performance liquid chromatography with ultraviolet-visible (HPLC-UV-Vis).



- 609** **N-Acetyl-cysteine Increases Chemical Stability of Hydroquinone in Pharmaceutical Formulations: a Theoretical and Experimental Approach**
 Rosivaldo S. Borges, Fernanda M. Costa, Tiago L. Pereira,
 Renata L. Araújo, Eduardo D. Almeida and
 Albérico B. F. da Silva

Graphical Abstract

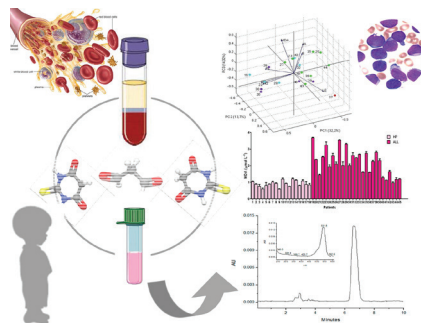
Chemical stability of hydroquinone (a) is compared to kojic (b). The hydroquinone was the most reactive. Its oxidation was inhibited more by N-acetylcysteine (d) than ascorbic acid (c).



- 615** **Evaluation of Oxidative Stress in Patients with Acute Lymphoblastic Leukemia: Experimental Evidence of the Efficacy of MDA as Cancer Biomarker in Young Patients**
 Mariana B. Almeida, Emanuel Carrilho and Suzana L. Nixdorf

Graphical Abstract

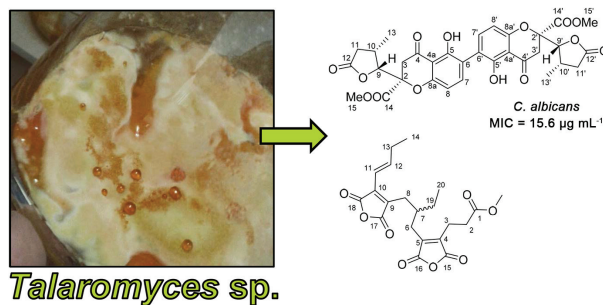
Malondialdehyde (MDA) efficacy as a cancer biomarker in acute lymphoid leukemia (ALL) that affects young patients was experimentally evidenced. Biochemical parameter charts associating with MDA contents, determined by high performance liquid chromatography, applying chemometric tools, allowed correlating risk stratification and assist in the disease diagnosis.



- 622** **Antifungal Polyketides and Other Compounds from Amazonian Endophytic *Talaromyces* Fungi**
 Paulo H. F. da Silva, Mayane P. de Souza, Eliana A. Bianco,
 Sarah R. S. da Silva, Liviane N. Soares, Emmanoel V. Costa,
 Felipe M. A. da Silva, Andersson Barison, Moacir R. Forim,
 Quezia B. Cass, Afonso D. L. de Souza, Hector H. F. Koolen
 and Antonia Q. L. de Souza

Graphical Abstract

Talaromyces fungi were isolated from Amazonian plants. From the antimicrobial extracts, 13 compounds were isolated and fully characterized by spectroscopic methods. Among the isolated compounds, polyketides, maleic anhydrides, and steroids were obtained, including two new compounds. The antifungal evaluation of the isolated compounds is described herein.



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C. albicans
 MIC = 15.6 µg mL⁻¹

631 Quality Assessment of Omega-3 Supplements Available in the Brazilian Market

Marília B. Galuch, Fabiana Carbonera, Thiago F. S. Magon, Roberta da Silveira, Patrícia D. S. dos Santos, Jessica S. Pizzo, Oscar O. Santos and Jesuí V. Visentainer

Graphical Abstract

Fish oil omega-3 supplements are eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) sources. However, fish oil is expensive raw material and its adulteration is common, especially with addition of edible oils with low cost, such as soybean oil. This study estimated the Brazilian reality regarding those supplements.

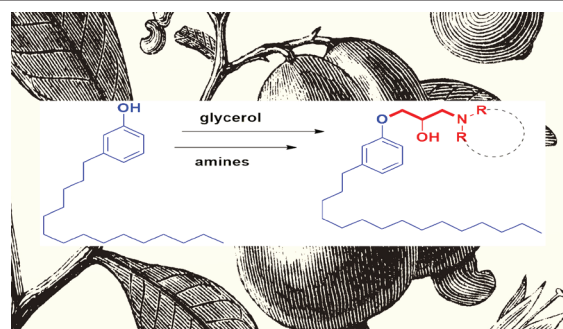


639 Synthesis, Antibacterial and Antitubercular Evaluation of Cardanol and Glycerol-Based β -Amino Alcohol Derivatives

Bhaskar R. Manda, Avvari N. Prasad, Narendar R. Thatikonda, Valdemar Lacerda Jr., Layla R. Barbosa, Heloia Santos, Wanderson Romão, Fernando R. Pavan, Camila M. Ribeiro, Edson A. dos Santos, Maria R. Marques, Dênis P. de Lima, Ana C. Micheletti and Adilson Beatriz

Graphical Abstract

Herein we provide a simple and efficient approach for the synthesis of amino alcohols by using cardanol and glycerol building blocks with amines under catalyst-free and mild conditions. Some of these synthesized compounds exhibited significant antimicrobial activity against *S. aureus* and *M. tuberculosis*.

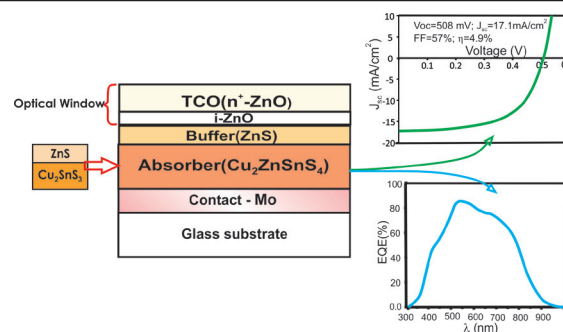


649 Novel Chemical Route for Deposition of $\text{Cu}_2\text{ZnSnS}_4$ Photovoltaic Absorbers

Gerardo Gordillo, Raul A. Becerra and Clara L. Calderón

Graphical Abstract

Solar cells with efficiencies of 4.9% were fabricated using a $\text{Cu}_2\text{ZnSnS}_4$ absorber layer synthesized following a novel chemical route based on the membrane assisted chemical bath deposition (CBD) technique.

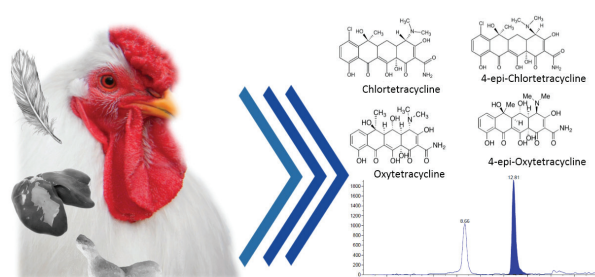


659 In-House Validation of HPLC-MS/MS Methods for Detection and Quantification of Tetracyclines in Edible Tissues and Feathers of Broiler Chickens

Ekaterina V. Pokrant, Aldo E. Maddaleno, Carolina E. Araya, Betty V. San Martín and Javiera Cornejo

Graphical Abstract

An in-house validation of methods was used for determination of tetracyclines in chicken feather, muscle and liver tissues, through high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS).



Additions and Corrections

669 Nano-Detoxification of Organophosphate Agents by PAMAM

Derivatives

*Esteban F. Durán-Lara, Fabian Ávila-Salas, Sebastian Galaz,
Amalraj John, Adolfo Maricán, Margarita Gutiérrez,
Fabiane M. Nachtigall, Fernando D. Gonzalez-Nilo and
Leonardo S. Santos*