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.

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Review

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

**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. Nogueira, Augusto Echegaray, 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. Candeloro 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

Graphical Abstract
Aerosol sampler installed at Tijuca sampling station, showing both EPA design PM$_{10}$ 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

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

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.
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 Jinhuo 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.
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.

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%.

Effect of Dy$^{3+}$ Amount on the Structural and Luminescence Properties of LaNbO$_4$:Dy$^{3+}$ 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 (Dy$^{3+}$)-LaNbO$_4$ 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, Nathalia Saib, 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

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

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

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 Cu₂ZnSnS₄ Photovoltaic Absorbers
Gerardo Gordillo, Raúl A. Becerra and Clara L. Calderón

Graphical Abstract
Solar cells with efficiencies of 4.9% were fabricated using a Cu₂ZnSnS₄ 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

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