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Cover Picture



Characterization of errors in multichannel analytical measurement vectors, in particular instrument noise, is important for understanding and improving experimental measurements and for the optimization of multivariate data analysis methods. This article reviews some of the techniques used to describe the interdependence of multivariate measurement errors, including error covariance/correlation matrices and frequency domain methods. Details are presented in the Account **Measurement Errors in Multivariate Chemical Data** by *Peter D. Wentzell* on page 183.

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Account

183 Measurement Errors in Multivariate Chemical Data Peter D. Wentzell



Graphical Abstract Graphical abstract illustrating the conversion of IR spectra of ink samples to a scores plot by making use of the error covariance matrix and maximum likelihood principal components analysis

Articles



PABA-MCM-41 synthesis procedure. Anew functionalized MCM-41-based mesoporous material was synthesized using a hydrothermal/cocondensation method. The CTAB surfactant was removed by refluxing in a solution of CH₃CH₂OH/HCl





Application of a Multivariate Exploratory Analysis Technique in the Study of Dissolved Organic Matter and Metal Ions in Waters from the Eastern Quadrilátero Ferrífero, Brazil Sl online Erik S. J. Gontijo, Francysmary S. D. Oliveira,

Mariana L. Fernandes, Gilmare A. da Silva, Hubert M. P. Roeser and Kurt Friese

Graphical Abstract

Some physico-chemical parameters and dissolved organic carbon data of waters of a mining region in southeast of Brazil were analysed using the multivariate technique Kohonen neural network. It provided a better visualisation and easier interpretation of the results



219 Using Chemometric Techniques to Characterize Gluten-Free Cookies Containing the Whole Flour of a New Quinoa Cultivar

Lilian M. Pagamunici, Aline K. Gohara, Aloisio H. P. Souza, Paulo R. S. Bittencourt, Alex S. Torquato, Weliton P. Batiston, Sandra T. M. Gomes, Nilson E. Souza, Jesuí V. Visentainer and Makoto Matsushita

Graphical Abstract

This study developed gluten-free cookies containing the whole flour of quinoa and linseed as source of essential fatty acids and minerals. The Principal Component Analysis (PCA) is a useful chemometric tool to facilitate the visualization of the best formulation





Shayessteh Dadfarnia, Ali M. Haji Shabani and Mahnaz Nozohor

Graphical Abstract

A DLLME-SFOD method based on the formation of the yellow Se(IV) complex with the 3,3'-diaminobenzidine (DAB) ligand combined with the spectrophotometry method was developed for the preconcentration, separation and determination of the inorganic selenium species



Characterization and Quantification by Gas Chromatography

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instrument

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Graphical Abstract

NMR experiments at lower temperatures and DFT(B3LYP/6-31G)/PCM methods were used to determine the 3D geometry of the favoured conformer of the macrocyclic ellagitannin oenothein B

Electrochemical Evidences of Linalyl Acetate (LA) Adsorption on Low-Carbon Steel in Aqueous and Ethanol Medium Fabiana N. Grosser, Tainá I. T. Barros and Reinaldo S. Gonçalves

Graphical Abstract

Linalyl acetate (LA): a chemical compound extracted from biomass and used as green corrosion inhibitor. Adsorbed species formed from LA adsorption on the metal surface inhibits the mechanism associated with the oxidation processes of the metal

298 Determination of Endocrine Disrupters and Pharmaceuticals in Sewage Samples by Tandem Solid Phase Clean up/Extraction and High Performance Liquid Chromatography-Negative and Positive Electrospray High-Resolution Mass Spectrometry Fernanda B. Queiroz, Júlio C. Silva, Sérgio F. Aquino, Maurício X. Coutrim and Robson J. C. F. Afonso

Graphical Abstract

Linear alkylbenzene sulphonates (LAS) occur in high concentration in raw sewage, thereof interfering with the analysis of micropollutants by mass spectromety. This paper proposes a tandem solid phase extractionprocedure that combines two distinct solid phase extraction cartridges to reduce LAS concentration in the extracts, thereby enhancing the sensitivity of the analytical method for the quantification of five pharmaceutical compounds and three endocrine disrupting chemicals in samples of raw and treated sewage

A Novel, Donor-Active Solvent-Assisted Liquid-Phase Microextraction Procedure for Spectrometric Determination



Wavelength / nm

Centrifugation

Extr

of Zinc Sl online Lívia Kocúrová, Ioseph S. Balogh, Martina Fatľová, Yaroslav Bazeľ, András Simon, Rastislav Serbin,

Miroslav Badida, Radoslav Rusnák and Vasil Andruch

Graphical Abstract

A donor-active solvent-assisted liquid-phase microextraction procedure followed by spectrophotometric determination of zinc was developed. The method is based on the ion associate formation between Zn(II), thiocyanate and 2-[2-(5-dimethylamino-thiophen-2-yl)-vinyl]-1,3,3trimethyl-3H-indolium bromide (DTVTI) reagent which is extractable by the mixture of toluene and tributylphosphate





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290

313

320

Biopolymer-Clay Nanocomposites: Cassava Starch and Synthetic Clay Cast Films Gustavo F. Perotti, Jairo Tronto, Marcos A. Bizeto, Celly M. S. Izumi, Marcia L. A. Temperini, Ademar B. Lugão, Duclerc F. Parra and Vera R. L. Constantino

Graphical Abstract

Polymer-clayfilms based on cassava starch and synthetic Laponite were prepared. Exfoliated nanocomposites are producedat low clay loadings. Starch crystallinitydecreases as the amount of Laponite is increased. Thermal decomposition profile is sensitive to the clay quantity in the hvbrid material





Helena Stecka, Dominika Jedryczko, Pawel Pohl and Maja Welna

Graphical Abstract

A simple and fast solid phase extraction sample preparation procedure for the flame atomic absorption spectrometry determination of traces of Cd, Co, Ni and Pb in honeys was proposed. The method provided the precision and the accuracy better than 4.5% and detection limits of 0.005 μ g g⁻¹ (Cd), 0.015 μ g g⁻¹ (Co, Ni) and 0.073 μ g g⁻¹ (Pb)



-19,0

-19.5 lecule⁻

-20,0

-20.5

-21,5

200

400

600

CH₃OH + Cl

800

т/к

s1)

In (k/cm³ -21,0

340 Ab Initio and CVTST Investigation of the Gas Phase Nucleophilic Substitution CH₃Cl + OH⁻ → CH₃OH + Cl⁻ Ana C. B. de Souza and Glauco F. Bauerfeldt SI online

Graphical Abstract

0

-10

-20

-30

-40

-50

-60

-70

CH₃CI + OH

AE / (kcal mol⁻¹)

In this work, the $CH_3Cl + OH \rightarrow CH_3OH + Cl$ reaction is investigated at the MP2/6-31+G(d) level and by the CVTST method. Final results for rate coefficients (1.94 \times 10 9 cm 3 molecule 1 s 1 at 298.15K) are found in agreement with the experimental data





Short Reports

 First Appraisal of Water Contamination by Antifouling Booster Biocide of 3rd Generation at Itaqui Harbor (São Luiz - Maranhão - Brazil)

Lia Gracy R. Diniz, Marcelle S. Jesus, Luis Alberto E. Dominguez, Gilberto Fillmann, Eny M. Vieira and Teresa Cristina R. S. Franco

Graphical Abstract

The Port of Itaqui (São Luís, Maranhão State, Northeast Brazil) stands out for heavy flow of vessels. Irgarol and Diuron are booster biocides present in antifouling paints and they were identified in such region that, jointly with north of Pará State, is located in the largest continuous mangrove area worldwide

