

CONTENTS

(Full texts are incorporated in CJELSEVIER, a file in the Chemical Journals Online database available on STN International; Abstracted, indexed in: Aluminium Abstracts; Anal. Abstr.; Biol. Abstr.; BIOSIS; Chem. Abstr.; Curr. Contents Phys. Chem. Earth Sci.; Engineered Materials Abstracts; Excerpta Medica; Index Med.; Life Sci.; Mass Spectrum. Bull.; Material Business Alerts; Metals Abstracts; Sci. Citation Index). Also covered in the abstract and citation database SCOPUS®. Full text available on ScienceDirect®.

Special Issue

Papers presented at the 10th International Conference on Chemometrics in Analytical Chemistry
Campinas, SP, Brazil, 10–14 September 2006

Editorial

Editorial

| | |
|--|-----|
| L. Buydens (Nijmegen, The Netherlands), M.M.C. Ferreira (Campinas, Brazil) and S. Rutan (Richmond, VA, USA) | 1 |
| Chemometric analysis applied in ¹ H HR-MAS NMR and FT-IR data for chemotaxonomic distinction of intact lichen samples G.B. Alcantara (São Carlos, Brazil), N.K. Honda (Campo Grande, Brazil), M.M.C. Ferreira (Campinas, Brazil) and A.G. Ferreira (São Carlos, Brazil) | 3 |
| MCR of the quenching of the EEM of fluorescence of dissolved organic matter by metal ions M.C.G. Antunes (Vila Real, Portugal), C.C.C. Pereira and J.C.G. Esteves da Silva (Porto, Portugal) | 9 |
| On the measurement of consistent long-term retention factor values in micellar liquid chromatography J.M. Bermúdez-Saldaña, L. Escuder-Gilbert, R.M. Villanueva-Camañas, M.J. Medina-Hernández and S. Sagrado (Valencia, Spain) | 19 |
| Mixture–mixture design for the fingerprint optimization of chromatographic mobile phases and extraction solutions for <i>Camellia sinensis</i> C.N. Borges, R.E. Bruns (Campinas, Brazil), A.A. Almeida and I.S. Scarmínio (Londrina, Brazil) | 28 |
| X-ray scattering and multivariate analysis for classification of organic samples: A comparative study using Rh tube and synchrotron radiation G.G. Bortoleto, S.S. de Oliveira Borges and M.I.M.S. Bueno (Campinas, Brazil) | 38 |
| Application of chemometric tools for automatic classification and profile extraction of DNA samples in forensic tasks I.T. Bustamante, F.S. Mata, N.H. González, R.G. Gazapo, J. Palau (Playa, Cuba) and M.M.C. Ferreira (Campinas, Brazil) | 43 |
| Application of genetic algorithm for selection of variables for the BLLS method applied to determination of pesticides and metabolites in wine R.L. Carneiro, J.W.B. Braga, C.B.G. Bottoli and R.J. Poppi (Campinas, Brazil) | 51 |
| Comparison of Plackett–Burman and supersaturated designs in robustness testing B. Dejaegher, M. Dumarey, X. Capron (Brussels, Belgium), M.S. Bloomfield (Surrey, UK) and Y. Vander Heyden (Brussels, Belgium) | 59 |
| Genetic algorithm optimisation combined with partial least squares regression and mutual information variable selection procedures in near-infrared quantitative analysis of cotton–viscose textiles A. Durand, O. Devos, C. Ruckebusch and J.P. Huvenne (Villeneuve d'Ascq, France) | 72 |
| Scale-up of batch kinetic models M. Ehly, P.J. Gemperline (Greenville, NC, USA), A. Nordon, D. Littlejohn, J.K. Basford and M. De Cecco (Glasgow, UK) | 80 |
| Chemometric study on the TiO ₂ -photocatalytic degradation of nitrilotriacetic acid C.A. Emilio, J.F. Magallanes and M.I. Litter (San Martín, Argentina) | 89 |
| How to avoid over-fitting in multivariate calibration—The conventional validation approach and an alternative N.M. Faber (Ede, The Netherlands) and R. Rajkó (Szeged, Hungary) | 98 |
| Multivariate near infrared spectroscopy models for predicting methanol and water content in biodiesel P. Felizardo, P. Baptista, J.C. Menezes and M.J.N. Correia (Lisbon, Portugal) | 107 |
| Non-destructive method for determination of hydroxyl value of soybean polyol by LS-SVM using HATR/FT-IR M.F. Ferrão (Santa Cruz do Sul, Brazil), S.C. Godoy, A.E. Gerbase (Porto Alegre, Brazil), C. Mello (Franca, Brazil), J.C. Furtado (Santa Cruz do Sul, Brazil), C.L. Petzhold (Porto Alegre, Brazil) and R.J. Poppi (Campinas, Brazil) | 114 |
| Study of the application of multiway multivariate techniques to model data from an industrial fermentation process A.P. Ferreira, J.A. Lopes and J.C. Menezes (Lisbon, Portugal) | 120 |
| Screening Brazilian C gasoline quality: Application of the SIMCA chemometric method to gas chromatographic data D.L. Flumignan, A.G. Tininis, F. de O. Ferreira and J.E. de Oliveira (Araraquara, Brazil) | 128 |
| Geographic origins and compositions of virgin olive oils determined by chemometric analysis of NIR spectra O. Galtier, N. Dupuy, Y. Le Dréau, D. Ollivier (Marseille, France), C. Pinatel (Aix-en-Provence, France), J. Kister (Marseille, France) and J. Artaud (Aix-en-Provence, France) | 136 |
| Improvement deoxyribo nucleic acid spots classification in polyacrilamide gel images using photometric normalization algorithms E.G. Llano, F.S. Mata, I.T. Bustamante, N.H. González and R.G. Gazapo (Playa, Cuba) | 145 |
| Complex numbers in chemometrics. Examples from multivariate impedance measurements on lipid monolayers P. Geladi (Umeå, Sweden), A. Nelson (Leeds, UK) and B. Lindholm-Sethson (Umeå, Sweden) | 152 |

| | |
|--|-----|
| Recognition of protozoa and metazoa using image analysis tools, discriminant analysis, neural networks and decision trees Y.P. Ginoris (Rio de Janeiro, Brazil), A.L. Amaral (Braga, Portugal and Bragança, Portugal), A. Nicolau (Braga, Portugal), M.A.Z. Coelho (Rio de Janeiro, Brazil) and E.C. Ferreira (Braga, Portugal) | 160 |
| X-ray spectrometry and chemometrics in sugar classification, correlation with degree of sweetness and specific rotation of polarized light K. Goraieb, T.L. Alexandre and M.I.M.S. Bueno (Campinas, Brazil) | 170 |
| The use of multivariate modelling of near infra-red spectra to predict the butter fat content of spreads P.C.M. Heussen, H.-G. Janssen, I.B.M. Samwel and J.P.M. van Duynhoven (Vlaardingen, The Netherlands) | 176 |
| Classification of perovskites with supervised self-organizing maps I. Kuzmanovski, S. Dimitrovska-Lazova and S. Aleksovska (Skopje, Macedonia) | 182 |
| Predicting the drug concentration in starch acetate matrix tablets from ATR-FTIR spectra using multi-way methods S. Matero, J. Pajander, A.-M. Soikkeli (Kuopio, Finland), S.-P. Reinikainen (Lappeenranta, Finland), M. Lahtela-Kakkonen, O. Korhonen, J. Ketolainen and A. Poso (Kuopio, Finland) | 190 |
| pH- and time-dependent hemoglobin transitions: A case study for process modelling G. Muñoz and A. de Juan (Barcelona, Spain) | 198 |
| Effect of missing values in estimation of mean of auto-correlated measurement series M. Paakkunainen, J. Kilpeläinen, S.-P. Reinikainen and P. Minkkinen (Lappeenranta, Finland) | 209 |
| A study of physicochemical and biopharmaceutical properties of Amoxicillin tablets using full factorial design and PCA biplot K.F.M. Pasqualoto, R.F. Teófilo, M. Guterres, F.S. Pereira and M.M.C. Ferreira (Campinas, Brazil) | 216 |
| Simultaneously calibrating solids, sugars and acidity of tomato products using PLS2 and NIR spectroscopy A.M.K. Pedro (Valinhos, Brazil and Caixa Postal, Brazil) and M.M.C. Ferreira (Caixa Postal, Brazil) | 221 |
| Alternative calibration approaches for LC-MS quantitative determination of coeluted compounds in complex environmental mixtures using multivariate curve resolution E. Peré-Trepat, S. Lacorte and R. Tauler (Barcelona, Spain) | 228 |
| Descriptive sensory analysis in different classes of orange juice by a robust free-choice profile method J. Pérez Aparicio, M. Ángeles Toledano Medina and V. Lafuente Rosales (Palma del Río (Córdoba), Spain) | 238 |
| Multivariate statistical analysis of a multi-step industrial processes S.-P. Reinikainen (Lappeenranta, Finland) and A. Höskuldsson (Kgs Lyngby, Denmark) | 248 |
| Spectroscopic on-line monitoring of reactions in dispersed medium: Chemometric challenges M.M. Reis (Porto Velho, Brazil), P.H.H. Araújo, C. Sayer (Florianópolis, Brazil) and R. Giudici (São Paulo, Brazil) | 257 |
| Factorial analysis of the trihalomethanes formation in water disinfection using chlorine P.M.S.M. Rodrigues (Guarda, Portugal), J.C.G. Esteves da Silva (Porto, Portugal) and M.C.G. Antunes (Vila Real, Portugal) | 266 |
| Self-modeling curve resolution (SMCR) by particle swarm optimization (PSO) H. Shinzawa (Hyogo, Japan and Changsha, PR China), J.-H. Jiang (Changsha, PR China), M. Iwashashi (Kanagawa, Japan), I. Noda (West Chester, OH, USA) and Y. Ozaki (Hyogo, Japan) | 275 |
| Direct determination of propranolol in urine by spectrofluorimetry with the aid of second order advantage L.C. Silva (Anápolis, Brazil), M.G. Trevisan, R.J. Poppi (Campinas, Brazil) and M.M. Sena (Anápolis, Brazil) | 282 |
| Application of non-linear optimization methods to the estimation of multivariate curve resolution solutions and of their feasible band boundaries in the investigation of two chemical and environmental simulated data sets R. Tauler (Barcelona, Spain) | 289 |
| Visualisation and interpretation of Support Vector Regression models B. Üstün, W.J. Melssen and L.M.C. Buydens (Nijmegen, The Netherlands) | 299 |
| Simultaneous multiresponse optimization applied to epinastine determination in human serum by using capillary electrophoresis L. Vera-Candioti (Santa Fe, Argentina), A.C. Olivieri (Rosario, Argentina) and H.C. Goicoechea (Santa Fe, Argentina) | 310 |
| On-line determination and control of the water content in a continuous conversion reactor using NIR spectroscopy H.W. Ward and F.E. Sistare (Groton, CT, USA) | 319 |
| Finding relevant spectral regions between spectroscopic techniques by use of cross model validation and partial least squares regression F. Westad (Oslo, Norway), N.K. Afseth (Ås, Norway) and R. Bro (Frederiksberg, Denmark) | 323 |
| Comparative analysis of volatile components from <i>Clematis</i> species growing in China Y.-X. Zeng, C.-X. Zhao, Y.-Z. Liang, H. Yang (Hunan, PR China), H.-Z. Fang (Heilongjiang, PR China), L.-Z. Yi and Z.-D. Zeng (Hunan, PR China) | 328 |