

## Monday, 30 June 2008

- 12:00 – 14:00 Registration
- 14:00 – 14:45 Conference opening
- 14:45 – 15:25 *Combining Analysis of Variance and PCA in the analysis of gene expression data* (L. Buydens)

### SESSION 1: NEW TRENDS IN CHEMOMETRICS

- 15:25 – 16:05 *A TRACE of chemometrics* (B. Vandegiste)
- 16:05 – 16:10 *Determination of the Shelf-Life of Cosmetics Using NIR Spectroscopy and the Multivariate Accelerated Shelf-Life Test* (A.K. Pedro)
- 16:10 – 16:30 *Likelihood ratio model for classification of forensic evidences* (G.Zadora)
- 16:30 – 16:50 *Visualization of quality parameters for classification of spectra in shooting crimes* (M. Otto)
- 16:50 – 17:10 Coffee break/Poster session 1
- 17:10 – 17:15 *Successive projection algorithm improving the classification of edible vegetable oils by using square wave voltammetry* (M.C.U. Araújo)
- 17:15 – 17:35 *Chemometric study of nanoparticles growth and conjugation* (J.M. Amigo)
- 17:35 – 17:55 *Support Vector Regression for Functional Data in Multivariate Calibration Problems* (N.H. González)
- 17:55 – 18:00 *Classification of Brazilian Soils by Using LIBS and Variable Selection in the Wavelet Domain* (C. Pasquini)
- 18:00 – 18:20 *A Comparative Study of Functional Data Analysis and Partial Least Squares for Calibration Modelling* (C. Jiang)
- 18:20 – 18:40 *Analysis of variance of complex data sets using GEMANOVA: An example using kill kinetics data* (D.B. Hibbert)
- 18:40 – 18:45 *Applied iPLS and siPLS regression models for quantification of metformin hydrochloride in pharmaceutical formulations using DRIFTS data* (E.I. Muller)
- 18:45 Welcome reception

## Tuesday, 1 July 2008

- 08:40 – 09:00 *Chemometrics of Ultrafast Time-resolved Spectra* (C. Ruckebusch)
- 09:00 – 09:05 *Optimization of DRIFTS-PLS models for the simultaneous quantification of sulphamethoxazole and trimethoprim in pharmaceutical formulations* (E.I. Muller)

### SESSION 2: METHOD DEVELOPMENT

- 09:05 – 09:25 *New proposals for PCA model building with missing data* (A.J. Ferrer)
- 09:25 – 09:45 *Chemometric Audits Through Perturbations and Permutations* (C.D. Brown)
- 09:45 – 09:50 *k-nearest neighbours classification with uncertainty in the variables* (J. Villa Medina)
- 09:50 – 10:00 Pause
- 10:00 – 10:20 *OPLS: an ideal tool for interpreting PLS regression models?* (H.S. Tapp)
- 10:20 – 10:25 *A new strategy for calibration transfer of MLR models based on the successive projections algorithm (SPA)* (C.F. Pereira)
- 10:25 – 10:45 *Multivariate Curve Resolution – Weighted Alternating Least Squares (MCR-WALS)* (R. Tauler)
- 10:45 – 11:30 Coffee break/Poster session 1

### SESSION 3: METHOD IMPROVEMENT AND ROBUSTNESS

- 11:30 – 12:00 *Adding value and safety to multivariate calibration by using the SBC approach* (R. Marbach)
- 12:00 – 12:20 *Increasing robustness against changes in the correlation structure by incorporating prior information in the Augmented Classical Least Squares (ACLS) framework* (W. Saeys)
- 12:20 – 12:40 *Measurement-Based Drift Correction in Spectroscopic Calibration Models* (P.S. Gujral)
- 12:40 – 12:45 *Determination of petroleum hydrocarbons in water by using IR spectroscopy and different multivariate calibration methods* (I.T. Bustamante)
- 12:45 – 13:05 *Prediction from Uncertain Inputs for PLS Regression* (E.B. Martin)- **CANCELLED**
- 13:05 – 13:25 *Contribution of EPO for calibration transfer in SW-NIRS - Application to gasoline quality* (S. Amat-Tosello)
- 13:25 – 13:30 *Total acid number determination in vacuum and atmospheric residue of crude oil using ATR-FTIR-PLS* (E.I. Muller)
- 13:30 – 14:30 Lunch
- 14:30 – 14:50 *Assessing measurement error structure and weighting in multivariate curve resolution*

*for time-resolved process data* (L. Blanchet)

- 14:50 – 15:10 *Estimation of Chemical Information in Latex Suspensions using Radiative Transfer Theory to Remove Multiple Scattering Effects* (R. Steponavicius)
- 15:10 – 15:30 *Tools for Multivariate Calibration Robustness Testing with Observations on Effects of Data Preprocessing* (B. Wise)
- 15:30 – 15:50 *Using ANOVA-PCA for variable selection and sample classification and replacing ANOVA by OSC to improve the detection of significant factors* (R.C. Pinto)
- 15:50 – 16:20 Coffee break/Poster session 1

#### **SESSION 4: DEVELOPMENTS IN PROCESS ANALYSIS**

- 16:20 – 17:00 *Process and Product Optimization using Latent Variable Models* (J. MacGregor)
- 17:00 – 17:20 *Fingerprints contribution plot: A new approach for fault diagnosis in multivariate statistic process control* (S. Vidal-Puig)
- 17:20 – 17:40 *Automatic Sample Weighting for Inferential Modeling of Historical In-Control Process Data* (J.M. Shaver)
- 17:40 – 18:00 *Using Scattering and Absorption Spectra as MCR-Hardmodel Constraints for Diffuse Reflectance Measurements of Tablets* (W. Kessler)
- 18:00 – 18:20 *Developments in Process Analysis that Extend Traditional Data Fitting to Non-Ideal, Industrially Relevant Processes* (M. Maeder)
- 18:20 – 18:40 *On-line monitoring of batch processes: Does the modelling structure matter?* (J. Camacho)- **Winner of the Massart Award**

Wednesday, 2 July 2008

**SESSION 5: PROCESS ANALYSIS APPLICATIONS**

- 08:40 – 09:10 *Process Analytical Technologies (PAT) tools for pharmaceutical process understanding and control – focusing on the science to achieve quality by design processes. Examples of applications, with special emphasis on "Chemometrics" (M. Zeiter)*
- 09:10 – 09:30 *Pharmaceutical process understanding: End-point detection by PLS-modeling (M. Kermit)*
- 09:30 – 09:50 *A chemometric approach to minimise the diffusive effect of the biomass when using near infrared spectroscopic measurements for the monitoring of bioprocesses (M. Lesteur)*
- 09:50 – 10:00 Pause
- 10:00 – 10:20 *Chemometrics Issues in Calibrating an On-Harvester Embedded NIR Sensor (C.R. Hurburgh)*
- 10:20 – 10:25 *Monitoring an activated sludge reactor using IR spectroscopy (J.A. Lopes)*
- 10:25 – 10:45 *On-line process near-infrared analyzer in Petrochemical : Assessment and Improvement of model robustness. Sharing problematics and Solutions with Agro-industries (S. de Lopez)*
- 10:45 – 11:40 Coffee break/Poster session 2
- 11:40 – 12:00 *Partial least squares estimation of mineral flotation slurry contents using optical reflectance spectra (O. Haavisto)*
- 12:00 – 12:20 *Rank augmentation of spectral reaction data using calorimetric and gas consumption data (N. Bhatt)*
- 12:20 – 13:00 Shoot out results
- 13:00 – 14:00 Lunch
- 14:00 – 18:30 Social event
- 20:00 Gala dinner

Thursday, 3 July 2008

## SESSION 6: -OMICS

- 09:15 – 09:55 *Chemometrics in metabonomics and metabolomics* (J. Trygg)
- 09:55 – 10:15 *Studies on special combinations of bases and relationships between the DNA primary sequences* (L. Xu)
- 10:15 – 10:25 Pause
- 10:25 – 10:45 *A new method for detection of differentially expressed genes: GAGG (Genetic Algorithm for Gene Gathering)* (F. Salipante)
- 10:45 – 11:05 *Self-Modeling Curve Resolution: a new approach to recovering temporal metabolite signal modulation in NMR spectroscopic data: Application to a life-long caloric restriction in dogs* (S.E. Richards)
- 11:05 – 11:25 *A new genetic algorithm in proteomics: 2D-gel electrophoresis alignment* (C. Reynès)
- 11:25 – 12:10 Coffee break/Poster session 2
- 12:10 – 12:30 *Chemometrics in proteomics* (B. Walczak)
- 12:30 – 12:50 *A multiway approach to data integration in genomics* (J.M. Prats-Montalbán)
- 12:50 – 13:10 *From Measurement to Knowledge: A Workflow for Multivariate Curve Resolution of Time Course DNA Microarray Data* (P.D. Wentzell)
- 13:10 – 13:30 *PLS Analysis with Gene Ontology data: inferring the phenotype from the function of genes* (A. Conesa)
- 13:30 – 14:30 Lunch
- 14:30 – 14:50 *Metabolites patterns in kidney transplant patients* (M. Calderisi)
- 14:50 – 15:20 *Statistical spectroscopy of metabolic supersystems* (J. Nicholson)

## SESSION 7: FOOD AND PHARMACEUTICAL APPLICATIONS

- 15:20 – 15:40 *Multiblock methods compare to Unfold and Standard methods. Application in origin prediction of virgin olive oil* (O. Galtier)
- 15:40 – 16:00 *MUBRE: an algorithm for multiblock regression. Application in sensory analysis* (M. Vivien)
- 16:00 – 16:20 *Multi-way analysis of chemometrically coupled UV and mass spectra for the semi-quantitative determination of the polyphenolic composition of red wines* (G. Mazerolles)
- 16:20 – 17:05 Coffee break/Poster session 2
- 17:05 – 17:25 *Study of the influence of micro-oxygenation and oak chip maceration on wine*

*composition using an Electronic Tongue (A. Rudnitskaya)*

- 17:25 – 17:45 *Prediction of antioxidant activity of Mallotus species from HPLC fingerprints (B. Dejaegher)*
- 17:45 – 17:50 *Application of chemometrics and FT-NIR spectroscopy in qualitative analysis of pharmaceutical preparations (M. Khanmohammadi)*
- 17:50 – 18:10 *Chemometrical tools to unravel hidden patterns in environmental monitoring data. Case of study: Tropospheric ozone in Catalonia (M. Felipe-Sotelo)*
- 18:10 – 18:30 *Chemometrics assisted diagnosis of malignant colon tissues by infrared microspectroscopy (A. Bagheri Garmarudi)- **CANCELLED***
- 18:30 – 19 :00 *Determination of Figures of Merit for Near-Infrared and Raman Spectrophotometers by Net Analyte Signal Analysis for a Four Compound Solid Dosage System (S.M. Short)- **Winner of the Büchi young scientist award***
- 19:00 Reception offered by Büchi (platinum sponsor of CAC2008)

Friday, 4 July 2008

#### SESSION 8: EXPERIMENTAL DESIGN

- 08:40 – 09:20 *Designs of experiments for robustness studies in analytical chemistry* (M. Sergent)
- 09:20 – 09:25 *An Experimental Design Approach Employing Artificial Neural Networks for the Determination of Potential Endocrine Disruptors in Food using Matrix Solid Phase Dispersion* (V.I. Boti)
- 09:25 – 09:45 *Statistical mixture design – varimax factor optimization for selective compound extraction from plant material* (R.E. Bruns)
- 09:45 – 09:50 *Experimental design application to extraction methods for epichlorohydrin determination in simulation liquids by HS-SPME and GC-ECD* (E. Millan)
- 09:50 – 10:00 Pause
- 10:00 – 10:20 *Development and optimization by design of experiments of a liquid chromatographic mass spectroscopy coupled method for the analysis of St John's wort compounds* (C. Delaurent)
- 10:20 – 10:25 *Determination of concomitants in thermospray flame furnace atomic absorption spectrometry (TS-FF-AAS) using background information* (E.R.P. Filho)
- 10:25 – 11:25 Coffee break/Poster session 2

#### SESSION 9: IMAGE ANALYSIS

- 11:25 – 12:05 *Multivariate and hyperspectral image analysis; overview and some special topics* (P. Geladi)
- 12:05 – 12:25 *Resolution of hyperspectral images. Pre-, in- and post-processing* (A. de Juan)
- 12:25 – 12:45 *Software analysis – Interactive tools for enhanced hyperspectral imaging analysis* (J. Burger)
- 12:45 – 12:50 *Selection of relevant pixels from NIR images to discriminate bovine vs porcine by-product meals, by near-infrared chemical imaging* (C. Riccioli)
- 12:50 – 13:10 *Angle Measure Technique (AMT) for image texture characterization - 10 years' development and application history* (K.H. Esbensen)
- 13:10 – 13:30 *Testing the homogeneity in pharmaceutical samples by NIR chemical image and multivariate analysis* (M. Bautista)
- 13:30 – 14:30 Lunch
- 14:30 – 15:00 *Advanced Approaches to Multivariate Curve Resolution Analysis of Hyperspectral Fluorescence Images* (D. Haaland)
- 15:00 – 15:20 *Kinetic Modeling of Multivariate Spectroscopic Images* (P. Gemperline)

- 15:20 – 15:40 *Comparison of MAF and PCA for Processing 3-D ToF-SIMS Images of Organic and Biological Samples* (B.J. Tyler)
- 15:40 – 16:00 *Optimization of probabilistic neurons networks in discrimination* (D. Bertrand)
- 16:00 – 16:40 Best poster and e-poster Awards & Best Junior Chemometrician Award
- 16:40 – 17:00 Closing session