

Scientific Program

Monday 11.6.2007

9.00 – 17.00 Courses

Tuesday 12.6.2007

Session 1: Chairman Satu-Pia Reinikainen

9.00 – 9.20 Opening

9.20 – 10.00 PL1: S. Wold: A Minimalistic approach to chemometrics.

10.00 – 10.20 O1: J. Trygg: Chemometrics philosophy and techniques for studying transgenic Poplar trees in functional genomics.

10.20 – 10.40 *Coffee*

10.40 – 11.00 O2: J. Gottfries: On the impact of nothingness in regression mathematics.

11.00 – 11.20 O3: M. Kermit: Assigning chemical information to NIR calibration models through L-PLS.

11.20 – 11.40 O4: H. Juhl: How to combine "slopy" y's

11.40 – 12.00 O5: F. Brakstad: Application and concept of value chain optimization.

12.00 – 13.00 *Lunch*

13.00 – 14.00 *Poster Session 1*

Session 2: Chairman Svante Wold

14.00 – 14.40 PL2: A. Höskuldsson: Path and Multi-block modeling.

14.40 – 15.00 O6: L. Eriksson: A new diagnostic for predictive models: OPLS-MANOVA.

15.00 – 15.20 O7: M. Bylesjö: Kernel-based orthogonal projections to latent structures (K-OPLS).

15.20 – 15.40 *Coffee*

15.40 – 16.00 O8: A. Lendasse: Optimal Linear Projection based on Noise Variance Estimation - Application to Spectroscopic Modeling -

16.00 – 16.20 O9: E. Alm: Vibrational overtone combination spectroscopy (VOCSY)—
a new way of using IR and NIR data.

16.20 – 16.40 O10: L. Blanchet: Multivariate Curve Resolution of Time Resolved Spectra.

16.40 – 17.00 O11: F. Corona: Using functional representations in spectrophotoscopic variables selection and regression.

Wednesday 13.6.2007

Session 3: Chairman Agnar Höskuldsson

9.00 – 9.40 PL3: O. Kvalheim: Analysis of Proteomic Profiles.

9.40 – 10.00 O12: T. Rajalahti: Pretreatment of mass spectral profiles: Application to proteomic data.

10.00 – 10.20 O13: T. Lundstedt: "Profiling of endogenous metabolites in spinal fluid - before and after a trauma".

10.20 – 10.40 *Coffee*

10.40 – 11.00 O14: L. Munck: Computerised data visualisation as a complement to data pre-treatment and chemometric tools for identification and interpretation of finely tuned reproducible spectral fingerprints in biological tissues.

11.00 – 11.20 O15: J. Cornel: Polymorph transformation monitoring using in-situ vibrational spectroscopy and chemometrics.

11.20 – 11.40 O16: M. Allesø: Solvent Diversity in Polymorph Screening.

11.40 – 12.00 O17: S. Caetano: Modelling the quality of enantiomeric separations using the Mutual Information as an alternative variable selection technique.

12.00 – 13.00 *Lunch*

13.00 – 14.00 *Poster Session 2*

Session 4: Chairman Johan Gottfries

14.00 – 14.40 PL4: J. Rantanen: PAT and chemometrics – future challenges for the pharmaceutical industry

14.40 – 15.00 O18: Å. Rinnan: Geometry optimizations effect on QSPR

15.00 – 15.20 O19: M. Ferreira: Quantitative Structure-Property Relationship (QSPR) study of phenolic passivation at the platinum electrode.

15.20 – 15.40 *Coffee*

15.40 – 16.00 O20: J. Camacho: Multi-Phase Analysis Framework for Handling Batch Process Data.

16.00 – 16.20 O21: T. Skov: Automated Preprocessing and Analysis of Chromatographic Data.

16.20 – 16.40 O22: R. Torgrip: Feature detection and alignment of LC/MS data. Inter- and intra-sample alignment of mass features using target tracking and clustering.

16.40 – 17.00 O23: G. Vivo-Truyols: Towards unsupervised analysis of second-order chromatographic data: Automated selection of the number of components in multivariate curve-resolution methods.

Thursday 14.6.2007

Session 5: Chairman Veli-Matti Taavitsainen

- 9.00 – 9.40 PL5: R. Carlson: Designed experiments in organic synthesis: Past, present, and future.
- 9.40 – 10.00 O24: B. Dejaegher: FEAR method to estimate factor effects in two-level supersaturated designs.
- 10.00 – 10.20 O25: P. Minkkinen: A Theoretical Study on Liberation Factor Defined in Gy's Sampling theory – Estimation of Fundamental Sampling Error.
- 10.20 – 10.40 *Coffee*
- 10.40 – 11.00 O26: O. Preisner: Estimation of uncertainty in microorganisms' discrimination.
- 11.00 – 11.20 O27: D. Muthas: Follow the lead – Focused Hierarchical Design of a Peptide Library targeted at *M. tuberculosis* Ribonucleotide Reductase.
- 11.20 – 11.40 O28: O. Rodionova: Simple View on Simple Interval Calculation (SIC) Method.
- 11.40 – 12.00 O29: I. Talavera: The use of Relevance Vector Machines for Multivariate Calibration purposes in Chemometrics.
- 12.00 – 13.00 *Lunch*
- 13.00 – 13.50 *Poster Session 3*

Session 6: Chairman Torbjörn Lundstedt

- 13.50 – 14.30 PL6: J. MacGregor: The interpretation of time varying medical images using latent variable and system identification methods.
- 14.30 – 14.50 O30: M. Otto: Sparse Matrix Computations for Classifications in Shooting Crimes.
- 14.50 – 15.10 O31: P. Teppola: Developing Optical Instruments: Computational Design Tools for Optical Instrumentation in Industrial Applications.
- 15.10 – 15.30 *Coffee*
- 15.30 – 15.50 O32: J. Prats-Montalban: Multivariate Image Analysis – based *Soft Sensors*: comparison of different approaches.
- 15.50 – 16.10 O33: K. Kvaal: A comprehensive database for (1-D, 2-D) texture and signal characterisation and the eAMTexplorer (Angle Measure Technique) software system.
- 16.10 – 16.30 O34: K. Esbensen: Optimal Corrections for Digitalization and Quantification Effects in Angle Measure Technique (AMT) Texture Analysis.
- 16.30 – 17.10 O35: K. Esbensen: The AMT Consortium: Resolving Two Generations of Angle Measure Technique Confusion.

Friday 15.6.2007

Session 7: Chairman Margret Thorsteinsdottir

- 9.00 – 9.40 PL7: H. Martens: Chemometrics and sensometrics for better mathematics in systems biology.
- 9.40 – 10.00 O36: F. Marini: More on Class-Modeling using Artificial Neural Networks.
- 10.00 – 10.20 O37: N. Grosej: The Use of FT-MIR Spectroscopy and Counter-Propagation Artificial Neural Networks for Tracing The Adulteration of Olive Oil.
- 10.20 – 10.40 *Coffee*
- 10.40 – 11.00 O38: J. Fernandez: Rapid and Non-Invasive Food and Feed Quality: The Chemometric Point of View.
- 11.00 – 11.20 O39: K. Lienemann: Automatic Toxicity Classification of ¹H-NMR Spectra from Rat Urine Using SVM-Ensemble.
- 11.20 – 11.40 O40: M. Cauchi: Chemometrics on a PDA.
- 11.40 – 12.00 O41: A. Astel: Multivariate modeling of environmental n-way data from bulk and throughfall precipitation quality control.
- 12.00 – 13.00 *Lunch*

Session 7: Chairman Pentti Minkkinen

- 13.00 – 13.20 O42: E. Mikhaylov: Landfill as Analytical Object. Part II. Chemometric approach.
- 13.20 – 13.40 O43: V-M. Taavitsainen: Ultrasonic Measurement of the Reaction Kinetics of the Setting of Calcium Sulfate Cements Using Implicit Calibration.
- 13.40 – 14.00 Closing