

FINAL PROGRAMME (UPDATED MAY 20)**SSC8****JUNE 14-18, 2003**

SATURDAY JUNE 14	
16.00-19.00	Registration
ca 19.30-	Get-together party
SUNDAY JUNE 15	
08.30-09.00	Annual Meeting of the Chemometric Division (in Swedish)
	SESSION I – PROCESS APPLICATIONS - BSPC Chairman: Lennart Eriksson, Organizing Committee
09.00-09.40 O1	<i>Multivariate modeling of batch processes</i> Nouna Kettaneh, Umetrics Inc, USA
09.40-10.05 O2	<i>Batch process diagnosis with PLS: variable selection versus hierarchical PCR</i> Manuel Zarzo, Polytechnic University of Valencia, Spain
10.05-10.30 O3	<i>Model predictive monitoring for batch processes with multivariate methods</i> Dora Kourti, MacMaster University, Hamilton, Canada
10.30-11.30	COFFEE / POSTERS & EXHIBITION
	SESSION 2 – PROCESS APPLICATIONS - MSPC Chairman: Dora Kourti, MacMaster University, Hamilton, Canada
11.30-11.55 O4	<i>Monitoring a paperboard machine using multivariate statistical process control</i> Anders Skoglund, Iggesund Paperboard AB, Sweden
11.55-12.20 O5	<i>Uncertainty intervals for monitoring statistics in MSPC with missing data using the trimmed scores estimator</i> Alberto Ferrer, Polytechnic University of Valencia, Spain
12.20-12.45 O6	<i>On non-stationarity in modelling dynamic systems</i> Satu-Pia Reinikainen, Lappeenranta University of Technology, Finland
12.45-14.00	LUNCH
	SESSION 3 – FOOD RESEARCH & SENSOMETRICS Chairman: Pentti Minkkinen, Lappeenranta University of Technology, Finland
14.00-14.40 O7	<i>Afraid of sensory data?</i> Magni Martens, The Royal Veterinary and Agricultural University, Denmark
14.40-15.05 O8	<i>An overview of applications of chemometrics in aquaculture research</i> Ragnar Nortvedt, University of Bergen, Norway
15.05-15.30 O9	<i>Fluorescence spectroscopy and PARAFAC in analysis of yoghurt</i> Jakob Christensen, The Royal Veterinary and Agricultural University, Denmark

15.30-16.30	COFFEE / POSTERS & EXHIBITION
	SESSION 4 – EMERGING CHEMOMETRICIANS – I Chairman: Kim Esbensen, Aalborg University Esbjerg, Denmark
16.30-16.55 O10	<i>Automated image analytical characterization of powder agglomeration by AMT-regression (Angle Measure Technique)</i> Casper Dahl and Lars Petersen, Aalborg University Esbjerg, Denmark
16.55-17.20 O11	<i>Multivariate monitoring of biological wastewater treatment plant A case study: Melbourne Water's Western Treatment Plant</i> Tarja Miettinen, Lappeenranta University of Technology, Finland
17.20-17.40	BREAK
17.40-18.05 O12	<i>PARAFAC and fluorescence</i> Åsmund Rinnan, The Royal Veterinary and Agricultural University, Denmark
18.05-18.30 O13	<i>Visualisation of skin impedance variations within volar forearms using parallel factor analysis</i> Peter Åberg, Karolinska Institutet, Sweden
	FREE EVENING
MONDAY JUNE 16	SESSION 5 – ORG SYNTHESIS & MEDICINAL CHEMISTRY/MEDICAL APPS Chairman: Johan Gottfries, Organizing Committee
09.00-09.40 O14	<i>Designs for explorative experiments in organic synthetic chemistry</i> Rolf Carlson, University of Tromsø, Norway
09.40-10.05 O15	<i>From peptides to low-molecular weight agonists – a multivariate story</i> Torbjörn Lundstedt, Melacure Therapeutics AB, Sweden
10.05-10.30 O16	<i>Medical applications of GC- and LC- MS and MS resolver</i> Olav Kvalheim, University of Bergen, Norway
10.30-11.30	COFFEE / POSTERS & EXHIBITION
	SESSION 6 – DRUG RELATED DESIGN AND QSAR Chairman: Torbjörn Lundstedt, Organizing Committee
11.30-11.55 O17	<i>Chemometric and molecular graphics and modeling study on bacterial β-Lactam efflux mechanism by multidrug resistance AcrB pump</i> Márcia Ferreira, Universidade Estadual de Campinas, Brazil
11.55-12.20 O18	<i>Biologically relevant chemical description - the quest for the Holy Grail!?</i> Peder Svensson, Carlsson Research AB, Sweden
12.20-12.45 O19	<i>Time-resolved QSAR: an approach to PLS modelling of three-way biological data</i> Lennart Eriksson, Umetrics AB, Sweden
12.45-14.00	LUNCH

	SESSION 7 – METABONOMICS, PROTEOMICS & BIOINFORMATICS Chairman: Henrik Antti, Metabometrix, Ltd, UK
14.00-14.40 O20	<i>Metabonomics and medicine: the biochemical oracle</i> Elaine Holmes, Imperial College, UK
14.40-15.05 O21	<i>Proteomics for target discovery</i> Johan Gottfries, AstraZeneca R&D, Sweden
15.05-15.30 O22	<i>Chemometrics methods for metabonomics in toxicology: constructing an expert system for the COMET project</i> Tim Ebbels, Imperial College, UK
15.30-16.30	COFFEE / POSTERS & EXHIBITION
	SESSION 8 – EMERGING CHEMOMETRICIANS - II Chairman: Svante Wold, Umeå University, Sweden
16.30-16.55 O23	<i>Multivariate characterization of excipient mixtures</i> Jon Gabrielsson, Umeå University, Sweden
16.55-17.20 O24	<i>Multivariate design, synthesis and biological evaluation of peptide inhibitors of PILUS assembly in pathogenic bacteria</i> Andreas Larsson, Umeå University, Sweden
17.20-17.40	BREAK
17.40-18.05 O25	<i>Exploratory analysis of ¹H-NMR data of monkey urine</i> Jeroen Jansen, University of Amsterdam, The Netherlands
18.05-18.30 O26	<i>Characterisation of genetically modified poplar using HR/MAS NMR and multivariate methods</i> Susanne Wiklund, Umeå University, Sweden
	FREE EVENING
TUESDAY JUNE 17	SESSION 9 – ENVIRONMENTAL MONITORING Chairman: Erik Johansson, Umetrics AB, Sweden
09.00-09.40 O27	<i>Chemometric application in environmental assessment of chemicals</i> Mats Tysklind, Umeå University, Sweden
09.40-10.05 O28	<i>Dependence of the bioaccumulation of PCDD/Fs and PCDEs in oligochaetes worms and semipermeable membrane devices on the molecular and sediment characteristics</i> Pentti Minkkinen, Lappeenranta University of Technology, Finland
10.05-10.30 O29	<i>Indicator parameters for PCDD/PCDF from electric arc furnaces</i> Tomas Öberg, Kalmar University, Sweden
10.30-11.30	COFFEE / POSTERS & EXHIBITION

	SESSION 10 – ANALYTICAL CHEMISTRY Chairman: Johan Trygg, Imperial College, UK
11.30-11.55 O30	<i>Chemometrics for multispectral imaging</i> Mats Josefson, AstraZeneca R&D, Sweden
11.55-12.20 O31	<i>Choosing the right calibration model – A new approach to an old problem</i> Geir Rune Flåten, The University of Hull, UK
12.20-12.45 O32	<i>Soft modeling for prediction of antioxidant activity in polypropylene</i> Oxana Rodionova, Semenov Inst of Chemical Physics RAS, Russia
12.45-14.00	LUNCH
	SESSION 11 – EMERGING CHEMOMETRICIANS - III Chairman: Harald Martens, MATFORSK, Norway
14.00-14.25 O33	<i>Quantification of lipoproteins in human blood plasma by 2D diffusion-edited NMR and three-way chemometric methods</i> Marianne Dyrby, The Royal Veterinary and Agricultural University, Denmark
14.25-14.50 O34	<i>The use of design of experiment and sensory analyses as tools for the evaluation of production methods</i> Gunilla Wormbs, Arla Foods AB, Sweden
14.50-15.20	COFFEE
15.20-15.45 O35	<i>Statistical experimental design, 'logical blocking' and time dependent metabolite response modeling for facilitating interpretation and understanding of METABONOMIC and other POST-GENOMIC data sets</i> Henrik Antti, Metabometrix, Ltd, UK
15.45-16.10 O36	<i>The effect of structured noise on latent variable regression (LVR) method, e.g. projections to latent structures (PLS)"</i> Johan Trygg, Imperial College, UK
18.00	CONFERENCE DINNER <i>Medal and Prize Ceremony:</i> Kowalski Prize for 2001 Emerging Chemometricians Awards 5 th Herman Wold Medal
WEDNESDAY JUNE 18	SESSION 12 – NEW APPLICATIONS IN CHEMOMETRICS - I Chairman: Olav Kvalheim, Bergen University, Norway
09.00-09.40 O37	<i>The utility of multivariate design in PLS modelling</i> Svante Wold, Umeå University, Sweden
09.40-10.05 O38	<i>Analysis of multi-block data</i> Agnar Höskuldsson, DTU Copenhagen, Denmark
10.05-10.30 O39	<i>New approaches for reliable industrial sampling and chemometric data analysis quality</i> Kim Esbensen, Aalborg University Esbjerg, Denmark

10.30-11.30	COFFEE / POSTERS & EXHIBITION
	SESSION 13 – NEW APPLICATIONS IN CHEMOMETRICS - II Chairman: Agnar Höskuldsson, DTU Copenhagen, Denmark
11.30-11.55 O40	<i>Visualization and outlier detection with Kernel PCA</i> Anton Belousov, Inst für Anorganische und Analyt Chemie, Germany
11.55-12.20 O41	<i>Some extensions of the PLS Regression</i> Harald Martens, MATFORSK, Norway
12.20-12.45 O42	<i>Complete two-component PLS factorization for process monitoring applications</i> Rolf Ergon, Telemark University College, Norway
12.45-14.00	CLOSING Final Words Svante Wold Torbjörn Lundstedt SSC8 Chairman of SSC9
14.00	LUNCH