SSC 10

10th Scandinavian Symposium on Chemometrics

June 11 – 15, 2007
Lappeenranta, Finland

www.lut.fi/kete/ssc10

Contents

How to Submit Your Manuscript

All presenters are invited to contribute to the SSC10 proceedings, which will be published in a special issue in *Journal of Chemometrics*. All the manuscripts will be peer reviewed in accordance with the editorial policy of *Journal of Chemometrics*, and the conference proceedings will be published as a separate volume in about one year after the SSC10.

Manuscripts for the proceedings should be submitted using Manuscript Central, Wiley's online journal submission tool. The web address for this tool is http://mc.manuscriptcentral.com/cem

All the authors should follow the instructions given, and at the bottom of the first page (Submit a Manuscript), when asked if the paper is for a special issue, they should select 'yes' from the dropdown menu and enter 'SSC10' when prompted for the special issue title.

All conference attendees will receive a free copy of the journal (the special issue) and they will have 3-months free online access from the publication date of the issue.

Preliminary deadline is June 15th, 2007.

Scientific Program

Monday 11.6.

9.00 – 17.00	Courses

Tuesday 12.6.

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.

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.

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.

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. Groselj: 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 ^{1}H-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

Registration (Main Hall of LUT)

Monday 11.6.:   8.00 – 9.00 and 18.00 – 20.00

Tuesday 12.6.:   8.00 – 9.00

Registration desk is open daily at 12.00-12.30 o'clock. Other times contact conference secretariat +358 5 621 7114 or ask LUT information desk to call Riitta Heiskanen.

Social Program

Social program for all participants and their accompanying persons:

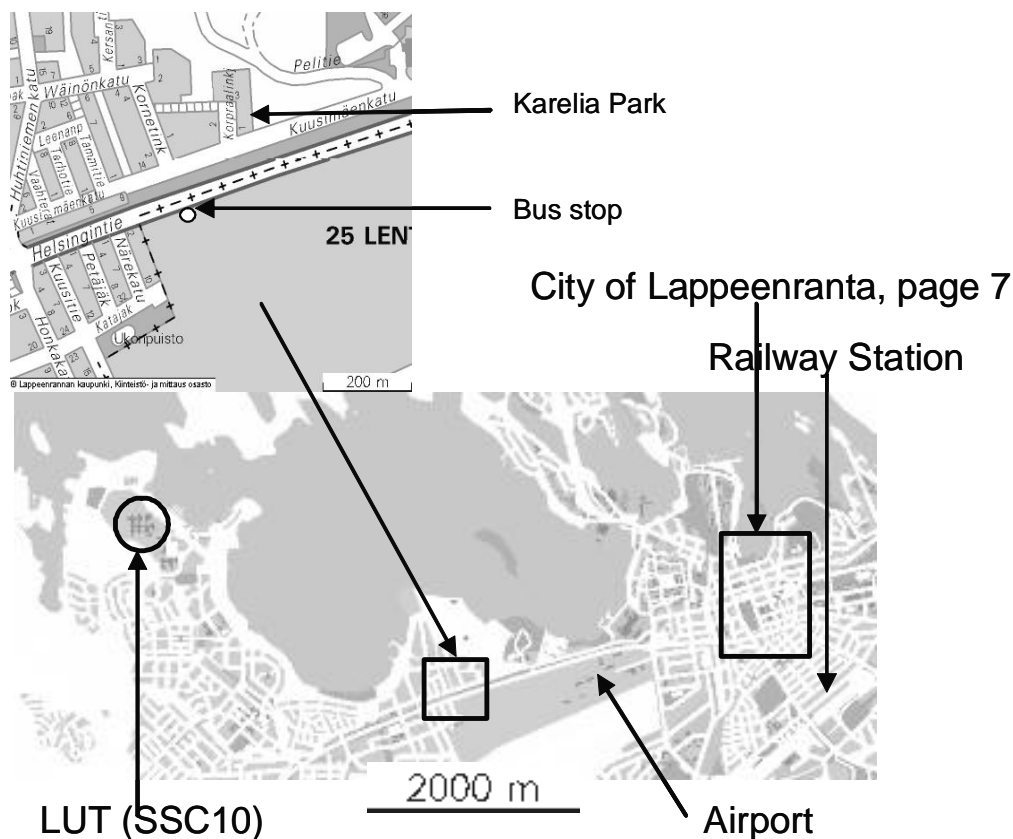|		
Monday 11.6.:	19.00 – 21.00	Get Together Party (Main Hall, LUT)
Tuesday 12.6.:	18.00 – 19.00	City Hall Reception
Tuesday 12.6.:	20.00 – 23.00	Sailing on Lake Saimaa
Wednesday 13.6.:	10.00 – 13.00	Sailing on Lake Saimaa
Wednesday 13.6.:	14.00 – 17.00	Sailing on Lake Saimaa
Wednesday 13.6.:	19.00 – 22.00	Sailing on Lake Saimaa
Thursday 14.6.:	19.00 –	Conference Dinner (Casino)

Accompanying persons: Special program is offered (museums, visit to stone village, etc). Please, give your contact phone at registration or contact Taina Haapasalo (+358 40 523 2126). Because of the low number of accompanying persons the program and schedule will be agreed during the conference.

Maps and instructions

Your conference bag includes map of Lappeenranta and some tourist information. In this leaflet you find instructions, how to reach different places.

How to get to LUT

Please, ask for a bus ticket from your hotel (Cumulus, Patria or Karelia Park). More tickets will be in your conference bag. They are valid in lines **1 and 5** from city of Lappeenranta to the University (LUT). The busses leave about every 20 minutes from the city (e.g., line 1 leaves from city at 15 and 45 minutes past every hour).
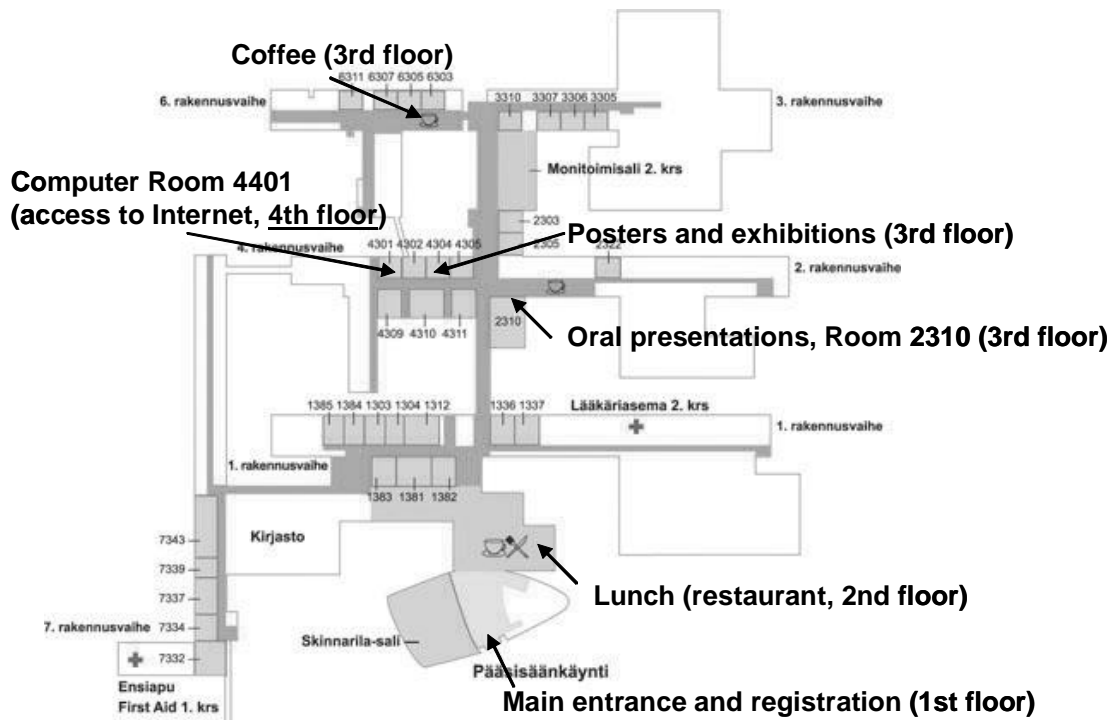

Karelia Park

Bus stop

City of Lappeenranta, page 7

Railway Station

25 LENT

200 m

© Lappeenrannan kaupunki, Kiinteistö- ja mittaus osasto

2000 m

LUT (SSC10)

Airport

Map: City of Lappeenranta

s/y Feie

Kasino

Scandic Patria

2 KESKUS 3 KYLPYLÄ

6 TA

Bus stop

Cumulus

City Hall

200 m

Map of Lecture Rooms

Coffee (3rd floor)

6311 6307 6305 6303

6. rakennusvaihe

3310 3307 3306 3305

3. rakennusvaihe

Monitoimisali 2. krs

Computer Room 4401
(access to Internet, 4th floor)

4301 4302 4304 4305

4. rakennusvaihe

2303

Posters and exhibitions (3rd floor)

2. rakennusvaihe

2310

4309 4310 4311

Oral presentations, Room 2310 (3rd floor)

1385 1384 1303 1304 1312

1336 1337

Lääkäriasema 2. krs

1. rakennusvaihe

1383 1381 1382

1. rakennusvaihe

7343

Kirjasto

7339

7337

Lunch (restaurant, 2nd floor)

7. rakennusvaihe 7334

7332

Skinnarila-sali

Ensiapu
First Aid 1. krs

Pääsisäänkäynti

Main entrance and registration (1st floor)

Bus stop

YO-talo

Sailing on Lake Saimaa (s/y Feie)

Lappeenranta is located next to Lake Saimaa, the fourth largest lake in Europe. The Saimaa drainage region covers most of the southern part of eastern Finland, a region about the size of Belgium. Saimaa is a labyrinthine watercourse, and there is 14 000 island in the region. There is a water canal from Lappeenranta to Vyborg bay, Russia.

The participants of SSC10 have a possibility to take a unique tour on Lake Saimaa. A sailing boat (a ketch), s/y Feie, will take the participants to see the beautiful nature and the lake. Feie has been originally built in Norway in 1932. It has renovated and accepted in museum register (traditional boats register).

The schedule of s/y Feie is on page 6. You should book your sailing trip, if you are interested in it (tour is free, and takes about 3 hours). The lists for each sailing tour can be found from the poster room or from registration desk, when it is open. The number of participants in each tour is limited to 12.

Exhibitors

Important Phone Numbers

Taxi (Lappeenranta)	+358 5 106 400
Emergency number (police, ambulance, etc.)	112
Conference Secretariat (Riitta Heiskanen)	+358 5 621 7114
Organizers (Satu-Pia Reinikainen)	+358 40 730 1851
Directory Enquiries	118 or 0 100 100