



Conferentia Chemometrica 2013

Sopron, Hotel Sopron
September 8-11, 2013



Chemometric Section, Hungarian Chemical Society
Automatic Analysis and Chemometric Working Group of the
Hungarian Academy of Sciences

Sunday evening, Sept. 08, 2013

16:00–19:00

Registration

19:00–21:00

Get-together party

Monday morning, Sept. 09, 2013

08:00–08:50

Registration

08:50–09:00

Opening, technical information

CHAIR: BAUMANN

Multivariate Data analysis; PLS Regression

09:00–09:30 L01 Agnar Höskuldsson: *Fine tuning of multi-block and path models*

09:30–10:00 L02 Kim H. Esbensen: *Quantifying 1- & 2-dimensional heterogeneity for reliable bulk analysis, process monitoring and multivariate calibration*

10:00–10:30

Coffee Break

CHAIR: Agnar Höskuldsson

Variable (feature) selection and cross-validation

10:30–11:00 L03 Knut Baumann, M. Busemann, A. ter Laak, N. Heinrich: *Cross-validation for large-scale QSAR models using time-dependent data*

11:00–11:30 L04 M. Cassotti, F. Grisoni and Roberto Todeschini: *Reshaped Sequential Replacement: an old approach to variable selection with new perspectives*

11:30–12:00 L05 Kurt Varmuza, P. Filzmoser, *Variable selection and its strict evaluation*

12:00–13:30

Lunch Break

Monday afternoon, Sept. 09, 2013

CHAIR: Todeschini

Method comparison, Ordering, Ranking, Correlation

13:30–14:00 L06 Lars Carlsen: *Partial order methodologies for chemometrics*

14:00–14:30 L07 Klára Kollár-Hunek, K. Héberger: *Approximation of probability distributions for sum of ranking differences with ties*

Calibration, Multivariate models

14:30–15:00 L08 Z. Dorkó, T. Verbić, György Horvai *Selectivity in analytical chemistry and chemometrics*

15:00–15:30 Coffee Break

15:30–16:00 L09 Róbert Rajkó, S. Beyramysoltan, H. Abdollahi: *Newer developments on self-modeling curve resolution (SMCR)*

16:00–16:30 L10 T. Natschläger, Birgit Zauner: *Transfer learning approaches for spectroscopic data*

16:30–17:00 L11 Milan Randić: *On some solved and unsolved problems in structure-property-activity studies*

17:00–18:00 Poster session

18:00–19:00 Wine tasting

20:00 Dinner

Tuesday morning, Sept. 10, 2013

'-Omics' world, applications

09:00–09:30 L12 Olav M. Kvalheim, E. Aadland, J. R. Andersen T. Rajalahti: *Life expectancy and lifestyle - What can metabolic profiling and latent variable regression models teach us?*

09:30–10:00 L13 Bjørn Grung, A. L. Hansen, M. Berg, M. P. Møen-Knudseth, G. Olson, D. Thornton, L. Dahl, and J. F. Thayer: *Investigating the effect of fatty fish consumption and medicinal use by multivariate analysis of heart rate variability data*

10:00–10:30 L14 Ivan Montoliu, M. Scherer, F. P. J. Martin, S. Collino, A. Rytz: *Improving feature extraction in -omics datasets*

10:30–11:00 Coffee Break

PLS discriminant analysis, Classification

11:00–11:30 L15 Richard G. Brereton: *Partial least squares discriminant analysis – taking the magic away*

11:30–12:00 L16 M. Bevilacqua, Federico Marini: *Local classification by locally weighted PLS-DA*

12:00–13:30 Lunch Break

Tuesday afternoon, Sept. 10, 2013

QSAR, Application, Optimization, Correlation

13:30–14:00 L17 J. Borišek, V. Drgan, N. Minovski, Marjana Nović, *Drug design of Cathepsin K inhibitors*

14:00–14:30 L18 Marjan Tušar, I. Ramljak, L. Avsenik, *A new approach to optimize the compaction of asphalt mixtures*

14:30–15:00 L19 Igor G. Zenkevich, *Precalculation of pKa values of substituted alkanecarboxylic acids using recurrent relations*

15:00–15:30 Coffee Break

Umetrics session

15:30–17:00 L20 Martin Berntsson, J. Hultman, *Making a valid prediction model with as few clicks as possible using spectroscopic data.*

L21 Johan Hultman, M. Berntsson, *Improved visualization and interpretation using OPLS and O2PLS with sensory and quality data*

L22 Johan Hultman, M. Berntsson, *Addressing, incorporating and visualization of risk in QbD*

17:00–18:00 Poster session

19:00– Conference Dinner (Distribution of the Best Poster Award)

Wednesday morning, Sept. 11, 2013

Session of the Automatic Analysis and Chemometric Working Group of the Hungarian Academy of Sciences:

09:00–09:30 L23 Gábor Járvas, J. Kontos, G. Nemeth, A. Dallos, *Temperature dependent surface tension estimation using COSMO-RS sigma moments*

09:30–10:00 L24 Brigitta Nagy, A. Farkas, B. Vajna, G. Marosi: *Linear and nonlinear regression methods in Raman mapping of homogeneous and heterogeneous two-component systems*

10:00–10:30 L25 Zoltán Nemes, N. Breza, S. Béni, F. Baska, C. Szántai-Kis, E. Illyés, Z. Horváth, D. Erős, E. E. Moret, P. Horváth, G. Kéri, L. Órfi: *The development and characterization of novel kinase inhibitors designed for targeted delivery*

10:30–11:00 Coffee Break

11:00–11:30 L26 János Elek, A. Mezósi, A. Rácz, *Estimation of active ingredient content by multivariate calibration: NIR examination of tablets used in ED treatment*,

11:30–12:00 L27 D. J. Kiss and Gergely Tóth: *Chemometric analysis of simulated evaporation trajectories*

12:00–14:00 Lunch

14:00– Departure

Poster sessions

Monday and Tuesday afternoon: 17:00–18:00

- P01 P. Ristivojević, Filip Lj. Andrić, J. Đ. Trifković, I. Dimikić, S. Stanković, Ž. Lj. Tešić, D. M. Milojković-Opsenica, Planar chromatography and multivariate image analysis in classification and modeling of antioxidative and antimicrobial activity of propolis extracts
- P02 Desiree Baumann, K. Baumann, Beyond Search-based Variable Selection: Predictivity, Model Selection and Stability
- P03 Tatyana Lj. Djaković-Sekulić, A.M. Smolinski, QSRR study of 5-arylidene-2,4-thiazolidinediones: stepwise multiple regression analysis for descriptors selection
- P04 Saioa Elcoroaristizabal, J.A. García, N. Durana, L. Alonso, J.L. Iardía, I. Elorduy, J. Iza, Chemometric determination of PAHs in aerosol samples
- P05 Attila Gere, D. Szabó, S. Kovács, K. Pásztor-Huszár, Z. Kókai, L. Sipos, Correspondence analysis of ranking data for creating preference maps of flavored kefir products
- P06 L. Sipos, Attila Gere, D. Szabó, S. Kovács, Z. Kókai, Multivariate methods for assessing sensory panel performance

- P07 **Károly Héberger**, S. Kolarević, M. Kračun, K. Sunjog, Z. Gačić, Z. Kljajić, M. Mitrić, B. Vuković-Gačić, Evaluation of single cell gel electrophoresis data: Combination of variance analysis with sum of ranking differences
- P08 **Károly Héberger**, Biljana Škrbić, Reevaluation of retention index models for alkybenzenes: Discrimination of equations via experimental data and consistency of predictive models
- P09 **Zoltán Herke**, T. Cserny, B. Magyar, Zs. I. Németh, Evaluation of enzyme kinetic data based on correlation and principal component analysis
- P10 **Éna Jakó**, N. Kézdi, Generalized molecular descriptors, algorithms and software (BOOL-AN) for chemo- and bioinformatic applications
- P11 **Norbert Kézdi**, É. Jakó, Molecular similarity analysis by using the ICF algorithm and graph distance calculations
- P12 **Dóra J. Kiss** and G. Tóth, The investigation of water evaporation with computer simulation
- P13 **Strahinya Z. Kovačević**, S.O. Podunavac Kuzmanović, L.R. Jevrić, N.D. Kalajdzija, E.S. Lončar, Molecular descriptors in chemometric analysis of TLC retention of some anhydropentose derivatives
- P14 N. D. Kalajdzija, S. O. Podunavac Kuzmanović, L. R. Jevrić, **Strahinya Z. Kovačević**, In silico ADME study of some benzimidazole derivatives and application of principal component analysis
- P15 **Krishna Chaitanya**, Bilal Malik and Mohammed Benaissa, Prediction of glucose concentration from near infrared spectra using local linear embedded regression combined with a digital band pass filter
- P16 **Sándor Kristván**, Statistical analysis of the electron-electron repulsion energy in the electronic Schrödinger equation via the coupling strength parameter, applications and tests with phospholipids
- P17 **Tibor Kulcsar**, Janos Abonyi, Genetic programming based visualization of NIR spectra – application to process monitoring
- P18 **Anikó Mezösi**, Ferenc Hámos, János Elek, Classification of original and counterfeit ED tablets by factor and discriminant analyses based on NIR spectroscopy data
- P19 **Lyudmila Naneva**, Ivan Bangov, Irini Doychinova, Marina Moskovkina, Employment of Descriptor Fingerprints in the QSAR Studies

- P20 Zsolt István Németh, R. Rákosa, R. Kocsis, D. Zs. Badáczy, Detection of pollution in groundwater with correlations of plant physiological variables
- P21 **Tamas L. Pap**, Mathematical description of long tailing peaks in capillary zone electrophoresis
- P22 Anita Rác, J. Elek, G. Papp, Multivariate data analysis of Hungarian spirit drinks' IR spectroscopic data
- P23 Zs. I. Németh, **Rita Rákosa**, Infrared spectrum of foliage as an indicator of interaction between plant and environment
- P24 **Biljana Škrbić**, Natasa Đurišić-Mladenović, N. Mačvanin, Comparison of the properties of diesel blends with biodiesel from edible and non-edible feedstocks
- P25 Francisco Torrens, G. Castellano, Classification of essential-oils components
- X P26 Kurt Varmuza, M. Dehmer, P. Filzmoser, Empirical modeling of mass spectral features by molecular descriptors
- P27 Špela Župerl, Katja Stopar, Marjana Nović, A data-driven model for the prediction of antiprion activity