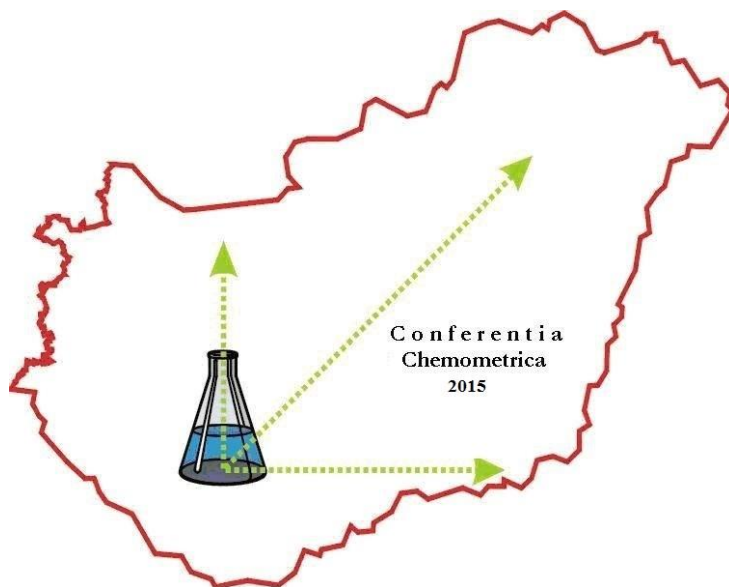




# Conferentia Chemometrica 2015

Budapest, MTA TTK  
September 13-16, 2015



**Research Centre for Natural Sciences  
Chemometrics and Chemoinformatics Working Group of the  
Hungarian Academy of Sciences**

# International Organizing Committee

**K. Héberger (Hungary) chair**

**K. Baumann (Germany)**

**R. G. Brereton (UK)**

**J. H. Kalivas (USA)**

**O. M. Kvalheim (Norway)**

**R. Todeschini (Italy)**

**K. Varmuza (Austria)**

## Local Organizers

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**Károly Héberger**, Research Centre for Natural Sciences, Hungarian Academy of Sciences

### Members:

**Dávid Bajusz**, Research Centre for Natural Sciences, Hungarian Academy of Sciences

**Anita Rácz**, Research Centre for Natural Sciences, Hungarian Academy of Sciences

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Edited by Károly Héberger

## Scientific Program of the Conferentia Chemometrica 2015: an overview

**Sept. 13, Sunday: 16:00–18:00 Registration 18:00–20:00 Get-together party; Sept. 14, Monday: 8:00-9:20 Registration, 9:20-9:30 Opening**

	Sept. 14, Monday		Sept. 15, Tuesday		Sept. 16, Wednesday
09:30 – 10:00	L01 R. Brereton	09:30 – 10:00	L12 T. Bączek	09:30 – 10:00	
10:00 – 10:30	L02 K. Baumann	10:00 – 10:30	L13 L. Kubik	10:00 – 10:30	L23 D. Bajusz
10:30 – 11:00	L03 I. Hoffmann	10:30 – 11:00	L14 A Voelkel	10:30 – 11:00	L24 J. Elek
11:00 – 11:30	Break	11:00 – 11:30	Break	11:00 – 11:30	Break
11:30 – 12:00	L04 R. Todeschini	11:30 – 12:00	L15 U. Maran	11:30 – 12:00	L25 G. Tóth
12:00 – 12:30	L05 J. Kalivas	12:00 – 12:30	L16 S. Cassani	12:00 – 12:30	L26 J. Simon
12:30 – 13:00	L06 R. Rajkó	12:30 – 13:00	L17 M. Hubert	12:30 – 13:00	L27 Z. Németh
13:00 – 14:00	Lunch	13:00 – 14:00	Lunch	13:00 – 14:00	Lunch
14:00 – 14:30	L07 O.M. Kvalheim	14:00 – 14:30	L18 K. Varmuza		<b>Departure</b>
14:30 – 15:00	L08 B. Grung	14:30 – 15:00	L19 I. G. Zenkevich		
15:00 – 15:30	L09 T. Lundstedt	15:00 – 15:30	L20 B. Debus		
15:30 – 16:00	Break	15:30 – 16:00	Break		
16:00 – 16:30	L10 G. Horvai	16:00 – 16:30	L21 V. Trivittayasil		
16:30 – 17:00	L11 M. Ferreira	16:30 – 17:00	L22 R. Gosselin		
17:00 – 18:00	<b>POSTER SESSION</b>	17:00 – 18:00	<b>POSTER SESSION</b>		
18:00 – 20:00	<b>Dinner Wine tasting</b>	19:00 –	<b>Banquet (Best Poster Award)</b>		

## Sunday evening, Sept. 13, 2015

- 16:00–18:00                      Registration  
18:00–20:00                      Get-together party

## Monday morning, Sept. 14, 2015

- 08:00–09:20                      Registration  
09:20–09:30                      Opening, technical information

### *Multivariate Data analysis, Classification*

- 09:30–10:00    L01 Richard G. Brereton:  
*Chemometrics: Fads and Fallacies*
- 10:00–10:30    L02 Knut Baumann, M. Mathea, W. Klingspohn:  
*The Applicability Domain for Classification Models*
- 10:30–11:00    L03 Irene Hoffmann, P. Filzmoser, S. Servels:  
*Sparse and Robust Partial Least Squares for Binary Classification*

- 11:00–11:30                      Coffee Break

### *Multivariate Data analysis, Classification, Novel Algorithms*

- 11:30–12:00    L04 Roberto Todeschini, D. Ballabio, M. Cassotti, V. Consonni:  
*N3 and BNN: Two New Similarity Based Classification Methods. An Extended Comparison with Other Classifiers*

### *Multivariate Calibration, Ranking, Novel Algorithms*

- 12:00–12:30    L05 John H. Kalivas, A. Tencate:  
*Fusion of Multiple Measures of Calibration Model Quality to Rank models Based on Multiple Tuning Parameters*
- 12:30–13:00    L06 Róbert Rajkó, H. Abdollahi, S. Beyramysoltan, N. Omidikia:  
*Definition, Description and Comparison of Data-based and Profile-based Uniqueness for Bilinear Chemical Measurements*

- 13:00–14:00                      Lunch Break

## Monday afternoon, Sept. 14, 2015

### *Partial Least Squares Regression, Theory, -Omics Applications*

- 14:00–14:30 L07 Olav M. Kvalheim:**  
*Predictive and Orthogonal Variation in Latent Variable Regression and Implications for the Concept of Model Quality and Model Reduction*
- 14:30–15:00 L08 Bjørn Grung, A. L. Hansen:**  
*Multivariate Investigation of the Effect of Nutrient Supplements on Norwegian Adolescents*
- 15:00–15:30 L09 Torbjörn Lundstedt, H. Shanker Sharma, T. Moritz, F. Troell, K. Bennett, K. Lundstedt-Enkel, and Johan Trygg:**  
*Endogenous Metabolic Profiling as a Fundament in Personalized Theranostics*
- 15:30–16:00** Coffee Break

### *Multivariate Selectivity, Calibration*

- 16:00–16:30 L10 Z. Dorkó, T. Verbić, George Horvai:**  
*Selectivity in (Analytical) Chemistry*

### *QSAR, QSRR, Novel Algorithms, Applications*

- 16:30–17:00 L11 Marcia M. C. Ferreira:**  
*LQTA-QSAR: a new 4D-QSAR Methodology*

- 17:00–18:00** Poster session  
**18:00–20:00** Dinner, Wine tasting

## Tuesday morning, Sept. 15, 2015

### *QSAR, QSRR, Novel Algorithms, (cont.) Chromatographic Applications*

- 09:30–10:00 L12 Tomasz Bączek, M. Belka, Sz. Ulenberg:**  
*Chemometric Analysis on Metabolic Stability of Drugs*
- 10:00–10:30 L13 Łukasz Kubik, P. Wiczling, M. J. Markuszewski, T. Bączek, E. Dagher-Wojtkowiak, R. Kaliszan:**  
*Quantitative Structure-Retention Relationships in Medicinal Chemistry and Laboratory Medicine*
- 10:30–11:00 L14 Z. Okulus, Adam Voelkel:**  
*Chemometric Implications to Inverse Gas Chromatography*

11:00–11:30 Coffee Break

*QSAR, Novel Algorithms, (cont.)*

11:30–12:00 L15 Uko Maran, S. Sild, V. Ruusmann, G. Piir, A. T. García-Sosa, K. Takkis, M. Oja, E. Laigna, P. Ahte, I. Kahn, A. Lomaka:

*QsarDB: Solution for Efficient Organization and Use of QSAR Models*

12:00–12:30 L16 Stefano Cassani, A. Sangion, E. Papa, P. Gramatica:

*Screening and Prioritization of Chemicals for REACH: modeling of Persistence, Bioaccumulation and Toxicity by the PBT Index*

12:30–13:00 L17 Mia Hubert, P. J. Rousseeuw, P. Segaert:

*Functional Outlier Detection for Image Data*

13:00–14:00 Lunch Break

**Tuesday afternoon, Sept. 15, 2015**

*Miscellaneous Applications*

14:00–14:30 L18 Kurt Varmuza, P. Filzmoser, M. Hilchenbach, I. Hoffmann, J. Silén:

*A Breeze of Chemometrics for Evaluation of Mass Spectra - Measured at Comet Dust Particles (On-board of Rosetta) and at Meteorite Samples*

14:30–15:00 L19 Igor G. Zenkevich:

*Mathematic Transformations of Recurrent Relations for Chemical Variables of Different Type's Homologues*

15:00–15:30 L20 Bruno Debus, D. Kirsanov, I. Yaroshenko, A. Sidorova, A. Piven, A. Legin:

*Quantitative Analysis of Urinary Creatinine with Common Electronic devices and PLS Regression*

15:30–16:00 Coffee Break

*Multivariate Curve Resolution*

16:00–16:30 L21 Vipavee Trivittayasil, T. Shoji, H. Kameya, M. Tsuta, M. Kokawa, J. Sugiyama:

*Estimation of Polyphenol and Procyanidins in Peach using Fluorescence Fingerprint*

**16:30–17:00** L22 **F. B. Lavoie, N. Braidy, Ryan Gosselin:**  
*LogLikelihood Multivariate Curve Resolution for Low-Count Spectral Image Analysis*

**17:00–18:00** **Poster session**

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

## **Wednesday morning, Sept. 16, 2015**

*Session of the Chemometrics and Chemoinformatics Working Group of the Hungarian Academy of Sciences:*

**10:00–10:30** L23 **Dávid Bajusz, A. Rácz, K. Héberger:**  
*Revival of an Old Debate: Cross- vs. external validation in QSAR modeling*

**10:30–11:00** L24 **János Elek, A. Simon, J. Török, A. Csontos, Cs. Ballai:**  
*Quantitative Application of Mid-Range Infrared Spectroscopy and Method Validation in GLP Environment*

**11:00–11:30** Coffee Break

**11:30–12:00** L25 **Gergely Tóth and G. Papp:**  
*Tuning of  $R^2$  by Test-training Allocation and a Grid Method for Splitting*

**12:00–12:30** L26 **J. Simon, A. Felinger:**  
*Correlation on 3D data – Alteration Analysis*

**12:30–13:00** L27 **Zsolt I. Németh, R. Rákosa, Z. Herke:**  
*Revealing Factor Effects on NIR Spectra of Alcohol-water Mixtures by Principal Component Analysis*

**13:00–14:00** Lunch

**14:00–** Departure

# Poster sessions

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

- P01** Filip Andrić, S. Šegan, A. Kosović, D. Milojković-Opsenica, Ž. Tešić, Modeling of Soil-water Partition Coefficient (logKOC) by Reversed-phase Thin-layer Chromatography
- P02** Filip Andrić, K. Héberger, How to Compare the Separation Performance of HPLC Columns Properly?
- P03** D. Zs. Badáczy, Zsolt I. Németh, Environmental Effects above Soil on Carbohydrate Levels of Forest Trees. Principal Component Analysis of Plant Carbohydrate and Environmental Data
- P04** A. Rácz, Dávid Bajusz, K. Héberger, Large Scale Statistical Comparison of Similarity Metrics for Fingerprint-based Calculations
- P05** Ewa Bartosińska, Ł. Kubik, D. Siluk, E. Dagher-Wojtkowiak, R. Kaliszan, P. Wiczling, QSRR Equations for Tocopherols' and Tocotrienols' Retention Prediction by Least Absolute Shrinkage and Selection Operator (LASSO) and HPLC Techniques
- P06** Stefano Cassani, F. Marzetta, P. Gramatica, Persistence Bioaccumulation Toxicity Assessment of Personal Care Products
- P07** A. Sangion, Stefano Cassani, P. Gramatica, Interspecies Quantitative Activity-Activity Relationships (QAAR) for pharmaceuticals
- P08** Stefano Cassani, A. Sangion, P. Gramatica, How to Avoid Dangerous Alternative to Banned Chemicals in a Safer Approach: Screening of Flame Retardants by the Cumulative PBT Index in QSARINS
- P09** Stefano Cassani, N. Chirico, A. Sangion, P. Gramatica, QSARINS: Software for the Development, Analysis and Validation of MLR Models and QSARINS-Chem: Insubria Dataset and QSAR models for Environmental Pollutants
- P10** Rafael Cela, S. Triñanes, C. Cobas, Pareto Optimality in the Quality-by-design Computer Assisted Optimization of Reverse-phase Liquid Chromatography Separations
- P11** Carlos Cernuda, E. Lughofer, T. Reischer, W. Kantner, M. Pawliczek and M. Brandstetter, Dynamically Slided Chemometric Models for Robust On-line Prediction of Cloud Point in Melamine Resin Production
- P12** Damian K. Chlebda, A. Majda, T. Łojewski, Discriminant Analysis of Writing Traces using Hyperspectral Imaging



- P13** Anna Dankowska, Detection of Chocolate Adulteration by Synchronous Fluorescence Spectroscopy with Multivariate Data Analysis
- P14** Viktor Drgan, Š. Župerl, M. Vračko, M. Novič, Artificial Neural Network Modelling of Fish Toxicity
- P15** Attila Eredics, Zs. I. Németh, R. Rákosa, E. Rasztovits, N. Móricz, P. Vig, Soil Moisture Sensitive State-dependent Correlations of Beach and Sessile Oak Leaf Reflectance Spectra
- P16** Mohammad H. Fatemi, E. M. Shahroudi, Development of Quantitative Interspecies Toxicity Relationship: Modeling of Chemicals to Fish
- P17** S. Kovačević, S. Podunavac-Kuzmanović, Slobodan Gadžurić, L. Jevrić, P. Jovanov, E. Djurendić, J. Ajduković Sum of Ranking Differences of QSRR Models. Case study: Prediction of Chromatographic Lipophilicity of  $17\alpha$ -Picolyl and 17(E)-Picolinylidene Androstane Derivatives
- P18** Attila Gere, L. Sipos, K. Héberger, Generalized Pair-wise Correlation Method for Development of Food Products
- P19** Attila Gere, L. Danner, N. de Antoni, S. Kovács, K. Dürschmid, L. Sipos, Comparison of Decision Times during an Eye-tracking Experiment
- P20** Sándor Kristyán, Toward the Prime Number Generator: Interesting Properties of Selector Functions  $2ab+a+b$  and  $6k_1k_2 \pm k_1 \pm k_2$  as well as a View from where the Distribution of Prime Numbers are not Erratic
- P21** Klára Kollár-Hunek, Károly Héberger, Classification of SRD-with-ties Probability Distributions
- P22** Zuzanna Okulus, A. Voelkel, Application of Chemometric Methods in Dental Fillings Stability Examination
- P23** Tamás L. Pap, Miklós Németh, Optimization of an Industrial Polymerization Process using Principal Component Analysis (PCA)
- P24** Anita Rácz, D. Bajusz, K. Héberger,  $n$ -class ROC Curves as Novel, Intuitive Tools for Method Comparison
- P25** Dalma Radványi, A. Gere, L. Sipos, S. Kovács, Zs. Jókai, P. Fodor, Application of HS-SPME-GC-MS Combined with Detrended Fluctuation Analysis to Distinguish Mould Species
- P26** Tatjana Đaković-Sekulić, Biljana Božin, Adam Smolinski Chemometric Study of Biological Activities of Lamiaceae Spices Essential Oils

- P27** Maryam Taraji, R. I. J. Amos, G. Schuster, M. Talebi, G. W. Dicoski, R. A. Shellie, P. R. Haddad, R. Szucs, J. W. Dolan, C. A. Pohl, HILIC method development in pharmaceutical analysis
- P28** Gyöngyi Vastag, S. Apostolov, B. Matijević, T. Đaković-Sekulić, Structure-retention Relationship Study of N-(4-phenylsubstituted) Cyanoacetamides by Multivariate Methods
- P29** Igor G. Zenkevich, A. N. Marinichev, Approximation of Octane Rating for Hydrocarbons of Different Series using Logistic Regression
- P30** Attila Farkas, B. Nagy, B. Démuth, P.L. Sóti, Z.K. Nagy, G. Marosi, Evaluation of Raman Mapping using MCR-ALS Equality Constraint in Stability Tests of Itraconazole Solid Dispersions
- P31** P. Rávai, Nikoletta Kerekes, J. Elek, Near Infrared Examination of Botanical Origin of Hungarian Honeys
- P32** M. Csontos, János Elek, Near Infrared Comparative Study of Hungarian Beer Market
- P33** Iiris Kahn, P. Ahte, G. Piir, S. Sild, U. Maran, Accessibility of Published QSAR models: Environmental Fate Endpoints
- P34** Eszter Ari, É. Jakó, Graph-based Generalized Boolean Descriptors for Classification of Biological Macromolecules
- P35** Zsófia Kovács, S. Balogh, É. Jakó, Analysis of Surface Water Quality Data by using Statistical Tools and a Novel Discrete Mathematical Approach
- P36** Péter Kunovszki, B. Bánfai, A. Deák, S. Kemény, Hypothesis Testing in Method Transfer
- P37** László Csaba Lengyel, T. Vágó, F. Darvas, Novel System for Rapid Identification and Characterization of Bacterial Organisms
- P38** Marjan Vračko, Regression Methods, Neural networks and Image Visualization for Early Forecast of Yield and crops