



**Conferentia
Chemometrica
2023**

**Sopron, Hungary
Hotel Sopron
September 10-13, 2023**



**Research Centre for Natural Sciences, Institute of
Excellence, Hungarian Academy of Sciences
Chemometrics and Chemoinformatics Working Group of the
Hungarian Academy of Sciences
Science Port Ltd**

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Edited by **Károly Héberger**

Scientific Program of the Conferentia Chemometrica 2023: an overview

Sept. 10, Sunday: 16:00–19:00 Registration 19:00–21:00 Dinner & get-together party;

Sept. 11, Monday: 8:30-9:20 Registration, 9:20-9:30 Opening

September 11 Monday		September 12 Tuesday		September 13 Wednesday	
09:30–10:00	L01 O.M. Kvalheim	09:30–10:00	L12 A. Tropsha	09:30–10:00	L23 K. Khan
10:00–10:30	L02 G. Tóth	10:00–10:30	L13 S. Podlewska	10:00–10:30	L24 M. Putz
10:30–11:00	L03 I.V. Tetko	10:30–11:00	L14 V. Poroikov	10:30–11:00	L25 A L. Pomerantsev
11:00–11:30	Break	11:00–11:30	Break	11:00–11:30	Break
11:30–12:00	L04 T. Andersons	11:30–12:00	L15 D. Kirsanov	11:30–12:00	L26 J. Abonyi
12:00–12:30	L05 S. Kovács	12:00–12:30	L16 B. Grung	12:00–12:30	L27 J. Hageman
12:30–13:00	L06 F. Andrić	12:30–13:00	L17 I. Stanimirova	12:30–13:00	L28 K. Héberger
13:00–14:00	Lunch	13:00–14:00	Lunch	13:00–14:00	Lunch
14:00–14:30	L07 T. Baczek	14:00–14:30	L18 M. Daszykowski	14:00–	Departure
14:30–15:00	L08 A. Farkas	14:30–15:00	L19 M. Csontos		
15:00–15:30	L09 A. Rácz	15:00–15:30	L20 L. Pieszczek		
15:30–16:00	Break	15:30–16:00	Break		
16:00–16:30	L10 R. Brereton	16:00–16:30	L21 J. A. Shimshoni		
16:30–17:00	L11 B. Vajna	16:30–17:00	POSTER SESSION		
17:00– 18:00	POSTER SESSION	17:00– 18:00			
18:00–19:30	Dinner	19:00-21:00	Banquet (Best Poster Award)		
19:30- 21:00	Wine Tasting				

Sunday evening, Sept. 10, 2023

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

Monday morning, Sept. 11, 2023

09:00–09:20 **Registration**
09:20–09:30 **Opening, technical information**

Latent variable regression, Seriation, Consensus modeling

09:30–10:00 **L01 Olav M. Kvalheim** Warren S. Vidar, Tim U.H. Baumeister, Roger G. Linington and Nadja B. Cech:
Confounding in model interpretation when using latent variable regression methods to make inferences

10:00–10:30 **L02 Gergely Tóth** and Rita Lasfar:
Patch seriation to visualize data and model parameters

10:30–11:00 **L03 Igor V. Tetko:**
Automatic detection of outlying compounds in the OCHEM platform using consensus modelling

11:00–11:30 **Coffee Break**

Ranking, multicriteria (multiobject) optimization, sum of ranking differences (SRD)

11:30–12:00 **L04 Tomass Andersons,** M. Sawall, K. Neymeyr:
Multivariate curve resolution with rank deficiency

12:00–12:30 **L05 Sándor Kovács,** Attila Gere, Károly Héberger:
Tailoring MultiCriteria Decision Making methods optimally for individual data sets

12:30–13:00 **L06 Filip Andrić:**
Multiobjective optimization of effect directed planar chromatography as a tool for fast screening of polypotent natural products

13:00–14:00 **Lunch Break**

Monday afternoon, Sept. 11, 2023

Data evaluation in chromatography, applications, metabolomics, chemical imaging, QSPR

- 14:00–14:30** **L07 Tomasz Bączek:**
Changes of fatty acids' levels in inflammatory bowel diseases in view of the samples collected within the Integrative Human Microbiome Project
- 14:30–15:00** **L08 Attila Farkas, Á. Kopasz, T. Jámbor, E. Varga, B. Nagy:** *Near-infrared and Raman chemical imaging for prediction of immediate dissolution of acetylsalicylic acid tablets*
- 15:00–15:30** **L09 Szilvia Klébert, Dóra Tátraaljai, Krisztina László, Anita Rácz:** *Prediction of physical and chemical features of structural materials with machine learning and classical chemometric tools*
- 15:30–16:00** Coffee Break
- 16:00–16:30** **L10 Richard G. Brereton:** *Features of Hotelling's T^2 on simulated and metabolomics data: A tutorial.*
- 16:30–17:00** **L11 Balázs Vajna:** *Data science: chemometric techniques generating business value*
- 17:00–18:00** **POSTER SESSION**
- 18:00–19:00** Dinner
- 19:00–21:00** Wine tasting

Tuesday morning, Sept. 12, 2023

Drug design, QSAR, consensus modeling

- 09:30–10:00** **L12 K. I. Popov, J. Wellnitz, T. Maxfield, and Alexander Tropsha:** *Hit Discovery using Docking ENriched by GEnerative Modeling (HIDDEN GEM): A Novel Computational Tool for Accelerated Virtual Screening of Ultra-large Chemical Libraries*
- 10:00–10:30** **L13 Agnieszka Wojtuch, Ewelina Jamrozik, Tomasz Danel, Sabina Podlewska:** *Explainability approaches in computer-aided drug design*

10:30–11:00 **L14 Vladimir Poroikov**, Dmitry Druzhilovski, Nadezhda Biziukova, Oleg Gomazkov, Alexander Veselovsky, Alexander Dmitriev, Sergey Ivanov, Nikita Ionov, Dmitry Karasev, Anastassia Rudik, Polina Savosina, Boris Sobolev, Leonid Stolbov, Vladislav Sukhachev, Olga Tarasova, Dmitry Filimonov: *Drug repurposing for Covid-19 therapy: in silico, in vitro, in vivo and in clinics*

11:00–11:30 Coffee Break

Green chemistry, applications, multivariate data analysis

11:30–12:00 **L15 Mikhail Saveliev**, Vitaly Panchuk, **Dmitry Kirsanov**: *The role of chemometrics in making analytical chemistry green*

12:00–12:30 **L16 Bjørn Grung**: *Characterizing solvent composition in a CO₂ capture plant using multivariate data analysis of online sensors and spectroscopic data*

12:30–13:00 **L17 Ivana Stanimirova** and P.K. Hopke: *A strategy for source apportionment analysis*

13:00–14:00 Lunch Break

Tuesday afternoon, Sept. 12, 2023

Chemometric modeling, statistical process control, hyperspectral chemical images, one class classification

14:00–14:30 **L18 Michal Daszykowski**, L. Pieszczyk, I. Stanimirova, S. Krzebietke, H. Czarnik-Matusiewicz: *Chemometric modelling of vital soil parameters*

14:30–15:00 **L19 Máté Csontos**, János Elek: *Needle in a haystack–NIR method development for quantifying novel foods and additives in rodent diet*

15:00–15:30 **L20 Lukasz Pieszczyk**, Michal Daszykowski: *Combining hyperspectral non-homogeneity measures and a one-class classification concept*

15:30–16:00 Coffee Break

16:00–16:30 **L21 Jakob Shimshoni**: *Near-Infrared Spectroscopy coupled with multivariate models to predict secondary metabolite and botrytis in cannabis and basil*

17:00–18:00 **POSTER SESSION**

19:00–

Banquet (best poster award)

Wednesday morning, Sept. 13, 2019

QSAR, QSPR, nanotoxicity, SIMCA

- 09:30–10:00** L23 Kabiruddin Khan, Agnieszka Gajewicz-Skretna: *The path of computational methods in assessing nanotoxicity: retrospective, current status, and future perspectives*
- 10:00–10:30** L24 Mihai V. Putz: *Balancing between antifragility and black swans in QSAR*
- 10:30–11:00** L25 Alexey L. Pomerantsev, O. Ye. Rodionova: *Mutter SIMCA und ihre Kinder [Mother SIMCA and her children]*
- 11:00–11:30** Coffee Break
- 11:30–12:00** L26 Martin Ferenczi, Ádám Ipkovich, Zsolt Tibor Kosztyán, János Abonyi: *Graph analysis based statistical process control*
- 12:00–12:30** L27 Jos Hageman, Carla Araya-Cloutier, Sylvia Kalli and Jean-Paul Vincken, *Validating QSAR models: an anti-MRSA case study*
- 12:30–13:00** L28 Károly Héberger: *The way it was: Personal, idiosyncratic reminiscences of past and present scientific achievements*
- 13:00–14:00** Lunch
- 14:00–** **Departure**

Poster sessions

Monday and Tuesday afternoon:

17:00–18:00

- P01** Mitra R. Alcaraz, M. Antonio, F. Chiappini, J. Zaldarriaga Heredia, S.M. Azcarate, J.M. Camiña, A. Muñoz de la Peña, M.J. Culzoni, H.C. Goicoechea: Higher-order data analysis to leverage the performance of food quality control procedures
- P02** Rosa Maria Alonso-Salces, G. E. Viacava, A. Tres, S. Vichi, E. Valli, A. Bendini, T. Gallina Toschi, L. A. Berrueta: Pattern recognition analysis of ¹H-NMR fingerprint data for the geographical authentication of virgin olive oils
- P03** Katharina Beier, T.-M. Dutschmann, P. M. Puttich, M. Lubienski, T. Beuerle, K. Baumann: Classification of horsetails using machine learning methods on NIR spectra
- P04** Bendegúz Borkovits, E. Kontsek, A. Pesti, S. Gergely, I. Csabai, A. Kiss, P. Pollner: Multivariate modelling of mid-infrared spectra of colorectal cancer
- P05** Máté Csontos, J. Elek, Z. Vincze: The effect of sample grinding in NIR spectroscopy
- P06** Pegah Dehbozorgi, L. Duponchel, V. Motto-Ros, Thomas Bocklitz: Laser-Induced Breakdown Spectroscopy (LIBS) data analysis
- P07** Tatjana Djakovic-Sekulić: Quantitative Structure–Retention Relationship study of β -tetralino-spiro-5-hydantoin derivatives
- P08** Pawel Dziki, L. Pieszczek, K. Rybicka, M. Daszykowski: Toward more efficient and effective color quality control in the large-scale printing process
- P09** J. Slezsák, Z. Gál, A. Salgó, Szilveszter Gergely: Investigation of carbohydrate powder mixtures by near-infrared spectroscopy and multivariate data analysis
- P10** Adriano A. Gomes, Ivan Špánik: Multiway one class classification PLS based
- P11** Dániel Kovács, Z. Fazekas: Sum of ranking differences (SRD) when differences diminish and reference ranking is ambiguous: the theoretical foundations of weighting schemes

- P12** Sándor Kovács, Károly Héberger: Selection of preferable and undesirable distance measures for stochastic optimization by cross entropy
- P13** Rita Lasfar and Gergely Tóth: The difference of model robustness assessment using cross-validation and bootstrap methods
- P14** Lilla Alexandra Mészáros, Attila Farkas, Zsombor Kristóf Nagy: Machine vision system and multivariate data analysis in the quality assessment of tablets
- P15** Nabiollah Mobaraki, K. Baumann: Non-membership probability for assigning a non-member (outlying) sample in different variants of random forest classification
- P16** Márton Mócz, P. P. Hanzelik, J. Slezsák, S. Gergely: Impact of different model transfer algorithms on dilution series and oil samples
- P17** Brigitta Nagy, A. Farkas, D. Galata, Zs. K. Nagy: Artificial neural networks in pharmaceutical process development and quality assurance
- P18** Anita Rácz, Anna Vincze, György T. Balogh: Extending the limitations in the prediction of permeability with machine learning algorithms based on a diverse PAMPA dataset
- P19** Oxana Ye. Rodionova, N. I. Kurysheva, G. A. Sharova, A. L. Pomerantsev: Chemometrics for personalized medicine
- P20** N. Tomčić, M. Jankov, P. Ristivojević, J. Trifković, Filip Andrić: High-performance thin-layer chromatography and multivariate image analysis in modelling of adulteration of *Salvia sp.* with olive leaves
- P21** Gyöngyi Vastag, S. Apostolov, Š. Ivošević: Chemometrics as a tool to monitoring corrosion degradation of the selected alloys in real conditions
- P22** Ekaterina Yuskina, Nikodim Makarov, Maria Khaydukova, Tatiana Filatenkova, Olga Shamova, Valentin Semenov, Vitaly Panchuk, and Dmitry Kirsanov: Contactless chemical analysis with high-frequency inductance coil and chemometrics
- P23** Kurt Varmuza, M. Dehmer, P. Filzmoser: Molecular descriptors based on automorphism data
- P24** Kurt Varmuza, P. Filzmoser: Adjusted Pareto scaling
- P25** N. Vladimirova, E. Puchkova, D. Dar'in, A. Turanov, V. Babain and D. Kirsanov: Application of quantitative structure-property relationship (QSPR) in predicting potentiometric sensor sensitivity to heavy metals

Posters

