

History

This meeting of Hungarian chemometricians will be the 36th in a row. The meeting has become international in 1997. The title of the conference has alternated: in odd years **Conferentia Chemometrica**, in even years **International Symposiums on Computer Applications and Chemometrics in Analytical Chemistry**. Now it is biannual. Selected papers of the conference appeared in *Chemometrics and Intelligent Laboratory Systems* (ACE&CC 2003, Vol. 72 No 2, CC2005 Vol. 87 Issue 1) and recently in *Journal of Chemometrics* (CC2007, Vol. 22 Nos. 3-4, SCAC2008 Vol. 23 No. 4, CC2009 Vol. 24. Nos 3-4, SCAC 2010 Vol. 25 No 5, CC 2011 Vol. 26 Nos 3-4. Vol. 28 No 4.) The locations were the following so far: Budapest (2003, 2007, 2010, 2012, 2015), Tihany (2004), Hajdúszoboszló (2005), Balatonalmádi (2008), Siófok (2009), Sümeg (2011) Sopron (2013) Budapest (2015)

Topics

Conferentia Chemometrica covers all aspects of chemometrics. Applications; Calibration; Classification; Cross-validation; Experimental design; Multivariate techniques; (ANN, HCA, CART, GA, LDA, MCR-ALS, MLR, PCA, QDA, PAT, PCR, PLS, RR, SVM, WFA, etc.) Metabonomics and Metabolomics; New algorithms; N-way data analysis; pattern recognition, Quality assurance; QSAR; QSPR; QSRR; Ranking, Spectroscopy; etc.

Invited Speakers (tentative titles)

Richard Brereton (England): Partial least squares discriminant analysis for chemometrics and metabolomics: how scores, loadings, and weights differ according to various interpretations

Michal Daszykowski (Poland): Monte Carlo validation of classification/discrimination models

Kim H. Esbensen (Denmark): Process Monitoring and Control – Chemometrics: TOS variography

Paul Haddad (Tasmania): Comparison of similarity measures for predicting retention in ion chromatography

Bahram Hemmateenejad (Iran): Screening for linearly and nonlinearly correlated variables in cheminformatics modeling

John H. Kalivas (USA): Reducing Ambiguity in Outlier Detection, Classification, and Forensics Image Analysis with Data Fusion

Lukasz Kubik (Poland): Determination of QSRRs with Bayesian Statistics

Dimitrii Kirsanov (Russia): Chemometrics for electronic tongue data processing

Olav Martin Kvalheim (Norway): Monte Carlo cross-validation for component selection and determination of prediction error in latent-variable regression

Marjana Nović (Slovenia): Antibacterial drug design – inhibition of peptidoglycan metabolising enzymes

Federico Marini (Italy): Chemometric modeling for traceability of apples cultivated in the Northeast Italy

Kunal Roy (India): Towards more precise predictions for external set compounds from multiple QSAR models

Ivana Stanimirova-Daszykowska (Poland): A modified weighted mixture model for the interpretation of compositional data

Beata Strzemieska (Poland): Chemometric evaluation of physicochemical characteristic of mesoporous materials

Roberto Todeschini (Italy): Chemometrics and ligand-based virtual screening: a new approach

Adam Voelkel (Poland): Application of solubility parameters in chromatography

Igor G. Zenkevich (Russia): Features of arguments' averaging in chemical relations. The role of additional standards in chromatographic quantification

Publication

Selected lectures (invited and submitted, oral or poster) will be published in a special issue of the

Journal of Chemometrics (Wiley)

after the normal refereeing process. Authors are cordially asked to submit their manuscript as soon as possible, during the conference or immediately after the conference via the Internet submission system. One of the reviewers will be chosen from the participants, if possible. Please follow the ethical guidelines of the American Chemical Society.

Poster session

Inspired by past years' success, poster contributions are encouraged. Best poster award will be awarded following the tradition (a cup with engravings). A Committee will decide on the best poster(s). The awards will be distributed during the banquet.

Accommodation

The participants will be accommodated in Hotel Szilvett or in the nearby Hotel of Károly Róbert University College (distance cca. 1.3 km from conference location). One-bed rooms at the conference location are assigned on a first-come first-served basis.

Location

Conferentia Chemometrica 2017 will be held in the conference room of

Hotel Sziluett, Farkasmály

Address:

H-3200 Gyöngyös-Farkasmály

Pincesor, hrsz: 067/47.

Phone: +36 37 309 074

GPS: 47.482183 19.572502



Rooms with bathroom
LCD TV cable channels
Mini bar
Safe
Free and unlimited WIFI Internet
Round-the-clock reception service
Free parking

Language

The official language of the conference is English.

Social Programs

Chemical singers concert (Sunday)
Wine tasting

Important dates and deadlines

Early bird registration: **June 15, 2017**

Abstract submission: **July 15, 2017**

Notification of acceptance: **August 1, 2018**

Payment: **August 16, 2017**

Registration: **August 16, 2018**

Conference: **September 03-06, 2017**

Manuscript submission:
September 31, 2017

Organizers

Research Centre for Natural Sciences,
Hungarian Academy of Sciences
Chemometric Section of the Hungarian
Academy of Sciences

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Conferentia Chemometrica 2017

**Gyöngyös, Farkasmály
Hungary
September 03-06, 2017**

Circular 1



Research Centre for Natural Sciences
Hungarian Academy of Sciences
Chemometric Section