

## History

This meeting of Hungarian chemometricians will be the 38th in a row. The meeting has become international in 1992. 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. 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 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, CC2011 Vol. 26 Nos 3-4, CC2013 Vol. 28 No 4, CC2015 Vol. 30 No 4, CC2017 Vol. 32 No 4). CC2022 Vol. 34 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), Gyöngyös (2017), Karcag (2019).

## Organizers

ELKH Research Centre for Natural Sciences,  
Institute of Excellence, Hungarian Academy  
of Sciences  
Chemometrics and Chemoinformatics  
Working Group of the  
Hungarian Academy of Sciences

## Social Programs

To be announced

## Confirmed speakers

**János Abonyi** (Hungary): Graph analysis based statistical process control

**Tomass Andersons** (Germany): Multivariate curve resolution with rank deficiency

**Tomasz Bączek** (Poland): Changes of short-chain fatty acids' levels in inflammatory bowel diseases in view of the samples collected within the Integrative Human Microbiome Project

**Richard Brereton** (UK): Features of Hotelling's T<sup>2</sup> on simulated and metabolomics data: A tutorial

**Michał Daszykowski** (Poland) et al.: Chemometric modeling of vital soil parameters

**Bjørn Grung** (Norway): Characterizing Solvent Composition in a CO<sub>2</sub> Capture Plant Using Multivariate Data Analysis of Online Sensors and Spectroscopic Data

**Sándor Kovács** (Hungary): Tailoring MultiCriteria Decision Making methods optimally for individual data sets

**Olav Kvalheim** (Norway): The good, the bad and the ugly

**Sabina Podlowska** (Poland): Explainability approaches in computer-aided drug design

**Vladimir V. Poroikov** (Russia): Drug repurposing for COVID-19 therapy *in silico*, *in vitro*, *in vivo* and in clinics

## Location

### Hotel Sopron, Sopron

Address:

H-9400 Sopron, Fővényverem u. 7.



## Important dates and deadlines

- Abstract submission: **July 31, 2023**
- Notification of acceptance: **August 07, 2023**
- Registration: **July 31, 2023**
- Payment: **July 31, 2023**
- Conference: **September 10-13, 2023**

## 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 (Anal. Chem. 2007, 79, 387–391).

## 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.

## The homepage of CC2023:

<http://cc2023.ttk.hu/>

## Scientific Secretariat:

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## Confirmed speakers (cont).

**Mihai Putz** (Romania): Balancing between Antifragility and Black Swans in QSAR

**Jakob Shimshoni** (Israel): Near-Infrared Spectroscopy coupled with multivariate models to predict secondary metabolite and botrytis in cannabis and basil

**Ivana Stanimirova-Daszykowska** (Poland): A strategy for advanced source apportionment analysis

**Igor Tetko** (Germany): Automatic detection of outlying compounds in OCHEM platform using consensus modelling

**Gergely Tóth** (Hungary): Patch seriation to visualize data and model parameters

**Alexander Tropsha** (USA): A novel Workflow for Hit Discovery using Docking ENriched by GEnerative Modeling (HIDDEN GEM)

**Adam Voelkel** (Poland): Resin-based composites as dental fillings. Application of chemometric techniques

Preliminary programme is now available and being updated at:

<http://cc2023.ttk.hu/programme.html>

This year's event is dedicated to **Prof. Károly Héberger**, head organizer of the **Conferentia Chemometrica** series, to celebrate his **70<sup>th</sup> birthday**.

# Conferentia Chemometrica 2023

An international conference on  
chemometrics and  
cheminformatics

**Sopron, Hungary**  
**Hotel Sopron**

**September 10-13, 2023**

## Circular 2



Research Centre for Natural Sciences  
Hungarian Academy of Sciences  
Chemometric Section  
Science Port Ltd