



Non-target screening of organic chemicals for a comprehensive environmental risk assessment

Congressi Stefano Franscini, Monte Verità, Ascona, Switzerland
29. May – 3. June, 2016

Image property of Congressi Stefano Franscini

Program

Sunday, May 29th, 2016

From 15.00	Arrival, check in, registration
17.00	<i>Welcome drink</i>
18.15 – 19.15	Derek Muir (Environment Canada) –Evening Lecture <i>Expanding the number of chemicals in commerce that can be determined in environmental media: a progress report</i>
19.30	<i>Dinner</i>

Monday, May 30th, 2016

8.15 – 8.30 **Chiara Cometta (CSF) and Lorenzo Sonognini (Monte Verità)**
Welcome address

Instrumentation and method development: Trends in LC-HRMS

8.30 – 9.00 **Nikolaos Thomaidis (Uni. Athens, GR) – Keynote Lecture**
Analytical strategies to explore the polar fraction of environmental samples by non-target LC-HRMS screening

9.00 – 9.20 **Thomas Letzel (TU Munich, DE)**
Novel suspects and non-target screening strategies for the simultaneous observation of very polar, polar and non-polar molecules in environmental (water) samples

9.20 – 9.40 **Juri Leonhardt (IUTA, DE)**
Development of a non-target time-of-flight mass spectrometric detection method for a miniaturized two-dimensional liquid chromatographic approach

9.40 – 10.00 **Martin Krauss (UFZ, DE)**
Teach your nontarget method new tricks: How retention at different pH and HDX improve compound identification by LC-HRMS

10.00 – 10.20 **Felix Hernandez (UJI, ES)**
Comprehensive investigation of organic (micro)pollutants in waters by GC and LC coupled to QTOF MS

10.20 – 10.50 *Coffee break*

Instrumentation and method development: Trends in GC-HRMS

10.50 – 11.20 **Eunha Hoh (SDSU, US) – Keynote Lecture**
An Analytical Framework for the Discovery of Bio-accumulative Organic Compounds

11.20 – 11.40 **Pablo Antonio Lara-Martin (Uni Cadiz, ES)**
APGC-ToF-MS for the determination of hydrophobic target and non-target contaminants in sewage impacted sediments

11.40 – 12.00 **Axel Rydevik (Uni. Bath, UK)**
Non-targeted analysis of wastewater by GCxGC-HRMS

12.00 – 12.20 **Merete Grung (NIVA, NO)**
Non-target and suspect identification of non-regulated polycyclic aromatic compounds and other markers of urban pollution in road tunnel particulate matter

12.30 *Lunch*

14.00 – 16.00 *Poster session*

16.00 – 16.30 *Coffee break*

16.30 – 18.00 **Workshops (details TBA)**

18.15 – 19.15 **David Wishart (Uni. Alberta, CA) – Evening Lecture**
Identifying the dark matter of the chemical exposome

19.30 *Dinner*

Tuesday May 31st, 2016

Workflow developments

- 8.30 – 9.00 **Steffen Neumann (IPB Halle, DE) – Keynote Lecture**
Hitchhiker's guide to computational mass spectrometry
- 9.00 – 9.20 **Gordon Getzinger (Duke Uni., US)**
Exploring environmentally relevant chemical space through ultrahigh resolution mass spectrometry, computational mass spectrometry and chemoinformatics: The example of wastewater derived organic micropollutants
- 9.20 – 9.40 **Christoph Ruttkies (IPB Halle, DE)**
MetFrag Relunched: Incorporating strategies beyond in silico fragmentation
- 9.40 – 10.00 **Saer Samanipour (NIVA, NO)**
Application of the unique ion extractor and dot product in suspect and target analysis of produced water
- 10.00 – 10.20 **Martin Loos (Eawag, CH)**
Spatiotemporal micropollutant monitoring with the LC-HRMS data mining workflow enviMass version 3
- 10.20 – 10.50 *Coffee break*

Tools to prioritize identification: Statistic and modeling

- 10.50 – 11.20 **Jan Christensen (Uni. Copenhagen, DK) – Keynote Lecture**
TBA
- 11.20 – 11.40 **Yaroslav Verkh (ICRA, ES)**
Derivation of information from non-target high resolution mass spectrometry (HRMS) analysis: statistical fingerprinting of organic content in waste water
- 11.40 – 12.00 **Aurea Chiaia-Hernandez (Eawag, CH)**
Temporal trend analysis on LC-HRMS measurements of lake sediments to prioritize organic contaminants
- 12.00 – 12.20 **Tobias Bader (Langenau, DE)**
General strategies to increase the repeatability in non-target screening by liquid chromatography-high resolution mass spectrometry
- 12.30 *Lunch*
- 14.00 – 16.00 *Poster session*
- 16.00 – 16.30 *Coffee break*
- 16.30 – 18.00 **Workshops (details TBA)**
- 18.15 – 19.15 **Mark Viant (Uni. Birmingham, UK) – Evening Lecture**
Applications of non-targeted metabolomics in environmental toxicology: workflows, challenges and routes through the maze
- 19.30 *Dinner*

Wednesday, June 1st, 2016

Transformation products in natural and technical systems

- 8.30 – 9.00 **Kathrin Fenner (Eawag, CH) – Keynote Lecture**
Transformation product analysis: Ready to go beyond suspect screening?
- 9.00 – 9.20 **Bozo Zonja (CSIC, ES)**
Data-dependent fragment ion search for detection of sartans and their related compounds in wastewater and surface water
- 9.20 – 9.40 **Jennifer Schollee (Eawag, CH)**
Gaining a comprehensive picture of transformation products formed during wastewater treatment processes
- 9.40 – 10.00 **Agneta Kiss (ISA, Lyon, FR)**
Non-target characterization and comparison of complex environmental samples: A practical example of pitfalls and benefits
- 10.00 – 10.20 **Dennis Vughs (KWR, NL)**
Tracing nitrogenous disinfection byproducts after medium pressure UV water treatment by stable isotope labeling and high resolution mass spectrometry
- 10.20 – 10.50 *Coffee break*
- 10.50 – 11.20 **Susan Richardson (U. South Carolina, US) – Keynote Lecture**
Non-target identification of new disinfection by-products
- 11.20 – 11.40 **Sylvain Merel (Uni. Tübingen, DE)**
LC-Q-TOF screening and Kendrick mass defect analysis for the identification of ozonation by-products
- 11.40 – 12.00 **Thomas Young (UCDavis, US)**
Assessing advanced oxidation reactor performance using high resolution mass spectrometry
- 12.00 – 12.20 **Damian Helbling (Cornell Uni., US)**
A non-target approach to identify chlorination products of sulfonamide antibiotics
- 12.30 *Lunch*
- 15.00 – 22.00 Excursion to Brissago Island and conference dinner

Thursday June 2nd, 2016

Linking to effects: Effect directed analysis, internal exposure

- 8.30 – 9.00 **Marja Lamoree (VU, NL) – Keynote Lecture**
Three pieces of the puzzle: advances in fractionation, toxicity testing and mass spectrometry for Effect-Directed Analysis
- 9.00 – 9.20 **Marie-Hélène Devier (Uni. Bordeaux, FR)**
Identification of unknown organic contaminants in wastewaters using Effect-Directed Analysis
- 9.20 – 9.40 **Audrey Buleté (ISA Lyon, FR)**
Non-targeted investigation of benthic invertebrates exposed to wastewater treatment plant effluents using nanochromatography coupled to high resolution mass spectrometry
- 9.40 – 10.00 **Martin Jones (Uni. Birmingham, UK)**
*Multi-platform non-targeted small molecule annotation of the ecological, eco-toxicological and freshwater model organism, *Daphnia magna**
- 10.00 – 10.20 **Nathan Dodder (SCCWRP, US)**
Methods and software for identification of contaminants in sentinel marine mammals
- 10.20 – 10.50 *Coffee break*

Non-target real world applications: Environmental samples

- 10.50 – 11.20 **Wolfgang Schulz (Langenau, DE) – Keynote Lecture**
Non-target screening using HPLC-HRMS in combination with Effect-Directed Analysis to prioritize contaminants in the aquatic environment
- 11.20 – 11.40 **Ana Causanilles (KWR, NL)**
Qualitative screening of new psychoactive substances in wastewater from a Dutch event using LC-HRMS
- 11.40 – 12.00 **Pablo Gago-Ferrero (SLU, SE and UoA, GR)**
Prioritization and identification of substances formed during wastewater treatment that are released into the aquatic environment
- 12.00 – 12.20 **Mark Strynar (EPA, US)**
Using point of use sampling devices and high resolution mass spectrometry techniques for characterizing drinking water exposures
- 12.30 *Lunch*
- 14.00 – 16.00 **Workshops (details TBA)**
- 16.00 – 16.30 *Coffee break*
- 16.30 – 18.00 *Workshop on demand*
- 18.15 – 19.15 *Workshops wrap up*
- 19.30 *Dinner*

Friday June 3rd, 2016

Applications & implications in a regulatory framework

- 8.30 – 9.00 **Heinz Singer (Eawag, CH)**
Routine non-target monitoring of river Rhine water quality: A Pandora's box?
- 9.00 – 9.20 **Uwe Kunkel (BfG, DE)**
Identification of quaternary triphenylphosphonium compounds as new class of environmental pollutants via non-target screening
- 9.20 – 9.40 **Annemieke Kolkman (KWR, NL)**
Elucidating the identity of a unknown contaminant in the river Meuse: Pyrazole, a new emerging polar industrial contaminant
- 9.40 – 10.00 **Georg Hanke (JRC, EU/IT)**
Marine contaminants – the need for analytical screening tools
- 10.00 – 10.20 **Jon Sobus (EPA, US)**
Harnessing high-throughput monitoring methods to strengthen 21st Century risk-based evaluations
- 10.20 – 10.50 *Coffee break*

Conference Wrap-Up

- 10.50 – 11.20 **Lee Ferguson (Duke Uni., US)**
Non-target 2016: Current challenges and future directions
- 11.20 – 11.35 CSF Award Ceremony
Flash presentation of award winner
- 11.35 – 12.00 Discussion and closing

12.15 Lunch and departure

For NORMAN Association Members and invited guests:

- 13.30 – 17.00 NORMAN Cross-Action Working Group Meeting on
Non-Target Screening (CA NTS)