

Report of the conference Nontarget2016

May 29 - June 3, 2016 at CSF, Monte Verità, Ascona, Switzerland

The conference NonTarget2016 addressed state-of-the-art non-target screening (NTS) approaches, including analytical technologies for detecting organic contaminants in environmental samples, application to real-world studies, and implementation in risk assessment. The main objective of the conference was to gather the best scientists from various, although related, disciplines to obtain different perspectives and better ideas on how to move NTS and its application forward in context of environmental analysis.

The conference with 120 participants from 21 countries worldwide brought together leading scientists from disciplines like environmental chemistry, informatics, food analysis and toxicology along with stakeholders from industry and regulatory bodies. Travel awards helped to bring more than 40 young researchers with fresh ideas to the venue thanks to different sponsors (Scopes, NORMAN Network, Swiss Society of Mass Spectrometry and the conference itself).

The program featured a mixed format with 3 plenary lectures and 8 keynote lectures from leaders in their fields along with 33 shorter oral and 62 poster presentations from conference participants. Two poster sessions on Monday and Tuesday afternoon facilitated the exchange of information and discussions. Additionally, 11 workshops (three in parallel, respectively) were organized in the afternoons by the conference organizers and further participants of the conference to stimulate intense discussions on the applicability of practical informatics tools as well as to trigger exchange of new and emerging strategies for unknown compound identification. In some workshops specific software or workflows were demonstrated, in others short presentations from participants or the workshop chairs stimulated the discussions. In a wrap-up session on Thursday before dinner the reports of the different workshops were presented to all conference participants. During the excursion to the Island Brissago on Wednesday afternoon and the various lunches and dinners, informal discussions about the conference topics took place.

The two plenary lectures from Mark Viant, UK and David Wishart, CA as well as a few presentations from participants showed nicely how the researchers in the field of non-target environmental analysis can learn from the more biological oriented and much larger fields of metabolomics and proteomics. The same technologies, i.e. mainly high resolution mass spectrometry, are applied and analogous databases of chemicals and mass spectra are in use and increasingly shared by both communities, especially for the common goal to identify the chemical exposome. The presentations of participants showed that for example metabolomics workflows such as XCMS, the spectra database MassBank as well as statistical tools like principle component analysis are already integrated in environmental applications. Presumably the environmental field will catch up fully in a few years and, in analogy to systems science in life sciences, environmental system science may become a reality. Compound databases such as STOFF-IDENT from Germany on chemicals with known environmental exposure with about 9,500 chemicals or the DSSTox chemical database from the US-EPA with more than 100,000 chemicals are increasingly used for a suspected screening in environmental samples.

The session "Instrumentation and method development" as well as a workshop on the topic on Monday demonstrated that new separation methods for polar or "difficult" compounds like HILIC, CE, SFC and two-dimensional GC and LC can be very powerful to separate chemicals with various properties. GC- and LC-HRMS methods along with different ionization techniques are used more often in concert to identify additional environmental contaminants and it was agreed this is essential to capture as many chemicals as possible.

The workflow session on Monday together with various workshops on specific software and workflows showed the trend for computational mass spectrometry that is facilitated by the increase of computer power and concurrently lower costs. This starts from rigorous cleaning of MS data with sophisticated algorithms such as in EnviMass, continues with the increased population of libraries like MassBank with clean HRMS spectra, and finally the weight-of-evidence identification including metadata (MetFrag 2.3) and the merge of MS and MSMS

information (Sirius, CSI:FingerID) for a more successful identification. In the future especially workflows applicable for also GC-HRMS with high energy ionization is needed. Despite the improvement of vendor software the trend goes to open-source tools which allow better comparisons across vendors and easy embedding of various meta information.

Inclusion of statistical approaches like replicate analysis and PCA are more and more successfully applied to distinguish relevant features from all the others. This was shown to be useful also in real-world applications such as wastewater and drinking water treatment and demonstrated to verify treatment effectiveness in removing contaminants.

The identification of transformation products (TPs) formed by biological or chemical processes in natural and technical systems was discussed during the entire Wednesday morning as many groups are working in this field and it is very relevant also for risk assessment. Since TPs can very often not be found in databases, identification has to go beyond database search. However, information from parent compounds such as specific fragments or time trends can be beneficial in the identification process. Pathway prediction tools like EnviPath and Biotransformer, presented by their inventors, can restrict the candidate pool. The presentation by Jennifer Schollée "Gaining a comprehensive picture of transformation products formed during wastewater treatment processes", that received the best oral presentation award, showed the inclusion of metabolic logic, PCA and hierarchical clustering into the workflow. Opening the analytical window provides also the opportunity for improved understanding of transformation mechanisms.

Proper prioritization is essential to perform an effective data analysis of the thousands of features revealed in chromatograms of complex environmental samples. Many approaches to prioritize such as frequency of occurrence or intensity thresholds were presented at the conference. Effect directed analysis using bioassays linked to sophisticated analytical tools for identifying "causative stressors" has advanced by coupling high-throughput testing methods to HRMS. For practical application in drinking water production, high performance thin layer chromatography (HPTLC) with on-plate assays was demonstrated as a surprisingly powerful approach for probing specific mechanisms. Nevertheless, several speakers also expressed that it is still difficult and time-consuming to assign "causality" and isolate stressors using effect-directed approaches. Internal dose measurement is critically important for establishing exposure and link effects to body burdens but still in its infancy.

During the last sessions real-world application on environmental samples including real-time monitoring and "contaminant forensics" was presented and put into a regulatory framework. The application of non-target screening in river monitoring was impressively demonstrated for the river Rhine in several studies in Switzerland, Germany and the Netherlands. NTS has advanced as a powerful forensic tool for finding contamination sources and triggering mitigation measures. Regulatory agencies have the opportunity to merge NTS with toxicity and exposure predictions in order to assess and ground-truth chemical risk. In the future regulatory programs such as REACH in Europe and TSCA (toxic substances control act) in North America can benefit from NTS to improve the registration process. Christoph Moschet, the winner of the CFS award for the best poster entitled "High-resolution mass spectrometry used to link effects on invertebrates in a vulnerable ecosystem" convincingly showed in his short talk on Friday morning during the closing session that it is even already possible to link NTS directly to environmental health.

Overall the feedback of the participants on the topics, structure and organization of the conference was extremely positive and a follow-up conference, possibly in North America in 2018, is envisaged to continue and foster international exchange and collaboration.

On behalf of all four organizers I like to thank all the sponsors and especially the SNF, ETH, and CSF which provided financial support and enabled a conference of high scientific value.

