International Conference on Non-Target Screening
(ICNTS 2021-Erding (Germany)

From 4th to 7th of October 2021, in Erding (a city close to Munich), Germany, the 1st International Conference on Non-Target Screening was held as a hybrid conference (face to face and online in parallel). Even though it was celebrated two and five years ago under a different name (SWEMSA), this year was the first with this title, comprising many different and new topics not present in the previous versions. The combination of face to face meeting and online attendance allowed to have 180 participants in these pandemic times, with 46 lectures and 34 scientific posters.

The overall aim of this meeting was to condense, standardize and harmonize various common aspects of non-target screening (NTS), to extend the use and understanding of software and workflow strategies and to learn about the potential of NTS applied in various disciplines. To do so, different main topics were selected and covered during the conference.

The congress started on Monday 4th with the welcome session, led by Prof. Thomas Letzel and Jochen Türk, organizers of the conference, who explained the entire path run from their first small project to the current conference project. Then, the first session about computational mass spectrometry was led by Prof. Emma Schymanski as chair and consisted of seven talks given by E. Bolton, Prof. S. Samanipour, X. Feng, A. Junior, R. Cariou, N. Meekel and R. Helmus. A panel discussion was held with all participants at the end of the session. Some of the speakers talked about software developed as PubChem (and all the possibilities that it offers to NTS), HaloSeeker (halogenated compounds detection) or patRoon (NTS workflows and transformation products (TPs) findings), but others focused on crucial ways to improveNTS from a computational way (as peak detection, peak picking, use of profile mode, alternatives in data treatment or prioritization of selected compounds for fragmentation). The second session in the afternoon was about metabolomics, with Michael Witting as chair. Speakers were Prof. W. Dunn, G. Tinnevelt, A. Lommen and R. Poulsen. Different matters were explained and discussed as features optimization and grouping, acquisition ways and modes, data storage and optimization of the space of this data or chemometric approaches in metabolomics.

Tuesday 5th started with the very interesting Environmental analysis session, with Leon Barron as chairman. He was the first speaker, followed by I. Fettig, M. Astudillo-Pascual, M.J. Farre, J. Sanchis and R. Gil-Solsona. Very different aspects in diverse sample types were discussed, as to what extent data has to be public and shared to everyone (or not) in the scientific community, but also to the rest of the community. Besides, biggest challenges of NTS in environmental samples, the importance of target-analysis or blank subtraction steps in specific cases were also discussed. In the afternoon, the next session about GC-MS and NTs in doping took place with Prof. Herbert Oberacher as chair. Prof. K. Jobst, A. Rebryk, V. Reinstadler, H. Oberacher and A. Thomas were the speakers and, initially, the discussion focused on the applicability of gas chromatography and how to adapt it to have more possibilities in NTS. Then, the discussion pointed out the difficulties that doping laboratories face and how NTS can help to identify new compounds and TPs of banned compounds, but also to retrospectively detect positives in old samples thanks to newly developed techniques.

After finishing the presentations, we had a guided tour around the city of Erding and the gala dinner afterwards.

Wednesday 6th started with Special chromatography meets NTS session with Jochen Tück as chair and the speakers were Prof. J. Quintana, K. Kochale, R. Romero-González and myself. We discussed among other

things, different approaches of chromatography and which ones were ideal in special cases with NTS applicability, but also which were the best combinations to have an efficient separation of the wider range of compounds possible. After this session, the Ion mobility meets NTS session started, with Lubertus Bijlsma as chair and the first speaker followed by T. Causon, L. Belova and F. Menger. The presentations noted many advantages about ion mobility and especially its applicability in NTS, and the discussion focused on matrix-independence in ion mobility, how to use CSS values for common use and if somehow a standard methodology can be used to report these values. Afterwards, the foodomics session started with Elke Richling as chair and speaker, followed by A. Knolhoff and R. Nijssen. The session focused on how NTS can be applied for food safety applications, looking for food contaminants with both liquid and gas chromatography, but also how workflows can be optimized for this purpose.

Thursday 7th was the last day of the conference, starting with Water analysis in NTS session, with Prof. Torsten Schmidt as chair and the first speaker, followed by Prof. C. Zwiener, R. Cunha, T. Köppe, G. Renner and M. Petri. This session was about some specific groups of compounds found in water, as PFAS or nitrosamines, but also to assess the big datasets in water analysis and how to standardize NTS processes. Afterwards, there was another very interesting session about NTS quality and tox transfer, with Herbert Oberacher as chair, and Prof. A. Kruve, S. Merel, S. Tisler, A. Sanchez Brotons, M. Sasse and C. Fisher as speakers. Many things were discussed in this long session, as quantification and toxicity prediction without standards, prioritization, toxicological examination, correction of matrix effects, and quality control strategies in NTS. To finish with the conference, it was said that it would happen again in 2023 and it would be held in Erding.

In summary, the conference time was very intense, with a big program condensed into three and a half days with plenty of high-quality sessions. Special mention about the quality of the posters in the congress that showed the big advances happening in NTS nowadays. I am so grateful for the opportunity to assist and present in this amazing congress, and I would like to encourage PhD students in the NTS field to assist in the next one in 2023. This opportunity would not have been possible without the travel support given by SECyTA, whom I would like to acknowledge and encourage to continue doing this great labor for its PhD students.

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