

## REPORT

### Training in application of dedicated software for non-target screening by HRMS

From 11<sup>th</sup> to 14<sup>th</sup> December 2023, two TwiNSol-CECs project team members from the Faculty of Technology Novi Sad (TFNS), Dr. Igor Antić and Dušan Rakić, Ph.D. student, visited Bremen (Germany) to participate in a 7<sup>th</sup> Compound Discoverer Users Meeting (12-13 Dec 2023). The travel, accommodation, and the participation fee were covered by an award received by Dušan Rakić during the Seminar „Advanced analytical techniques in food, environment & pharma“ organized by Analysis doo company from Belgrade, a certified retailer of Thermo Fisher Scientific equipment in Serbia. This was a great opportunity for TFNS young researchers to learn more about high resolution mass spectrometry (HRMS) and its deployment in advanced non-target analysis as a powerful tool for the wide-range surveillance of chemicals in the environment.

Thermo Scientific Compound Discoverer™ (CD) is a dedicated software, which purchase together with a powerful computer was enabled by TwiNSol-CECs budget, and it enables high resolution mass spectrometric (HRMS) data processing, which has been enabling non-target analysis by the existing UHPLC-HRMS instrument (based on Orbitrap technology, Exactive) at TFNS<sup>1</sup>.

During the two days of the meeting, Thermo's experts gave valuable lectures to the invited CD software active users regarding the latest improvements of CD software, its application, and its wide ability for applications in different fields including the analysis of different toxic pollutants in environmental samples. The participants also had a great honor of hearing the presentation on the latest improvements in analytical instruments that are compatible with the CD software held by Prof. Dr. Alexander Makarov, a Director of Research at the Life Science Mass Spectrometry Business Unit of Thermo Fisher Scientific located in Bremen, a physicist who led development of the Orbitrap-based mass spectrometer (Exactive™, OrbitrapFusion™, Q Exactive™) that generates HRMS data to be used for identification of compounds during suspected or unknown screening analysis.

The main objectives of the meeting were:

- to bring beginners up-to-speed with the best practices
- to allow advanced users to interact with software experts and learn how to get the most out of their data
- to learn about recent developments and new technologies
- to meet other users and learn how they are using Thermo Scientific Compound Discoverer including applications

The lectures dedicated to CD software included:

- Performance improvements and database updates in CD 3.3. SP3
- Updates on spectral libraries and automated method building
- Best kept secrets of CD
- Complimentary of GC- and HPLC-HRMS data evaluation using CD
- Molecular Networking in CD
- Getting the best results of users' raw files: acquisition strategies

<sup>1</sup> [https://twinsol-cecs.com/images/documents/r3\\_2-instalation-of-compound-discoverer\\_jan\\_2023.pdf](https://twinsol-cecs.com/images/documents/r3_2-instalation-of-compound-discoverer_jan_2023.pdf)

- Experimental design, data acquisition, and -processing for successful application of CD
- Discussion with the experts

At the end of the second day, the organizers managed a Thermo’s mass spectrometry factory tour. It was a great opportunity for the participants to familiarize themselves with the HRMS production path.



**Figure 1.** Dušan Rakić (up right) and Dr. Igor Antić (middle right) at the 7<sup>th</sup> Compound Discoverer Users Meeting, 12-13 December 2024; this was an opportunity to meet eminent Prof. Dr. Makarov, who led development of Orbitrap-based HRMS technology (down right)

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