REPORT:

4th TwiNSol-CECs Training

"*Target and suspect screening of CECs present in surface water samples*"

Spanish National Research Council, Institute of Environmental Assessment and Water Research (CSIC), Barcelona, Spain

8-12 May 2023

The fourth onsite TwiNSol-CECs Training was organized as a one-week visit of three researchers from the Faculty of Technology Novi Sad (TFNS) at the partner institution - the Spanish National Research Council, Institute of Environmental Assessment and Water Research (CSIC), Barcelona, Spain, in the period May 08-12, 2023. The agenda of the 4th TwiNSol-CECs Training is an integral part of this report. The training was a part of activities within the TwiNSol-CECs project (101059867) Work Package 3 "Reinforcing research knowledge and skills of TFNS of TwiNSol-CECs project". It was organized as a joint training and research event attended by TFNS team members, Dr. Jelena Živančev, Dr. Igor Antić, and Dušan Rakić, PhD student, and the whole CSIC research team led by Dr. Marinella Farre, CSIC Project Manager.

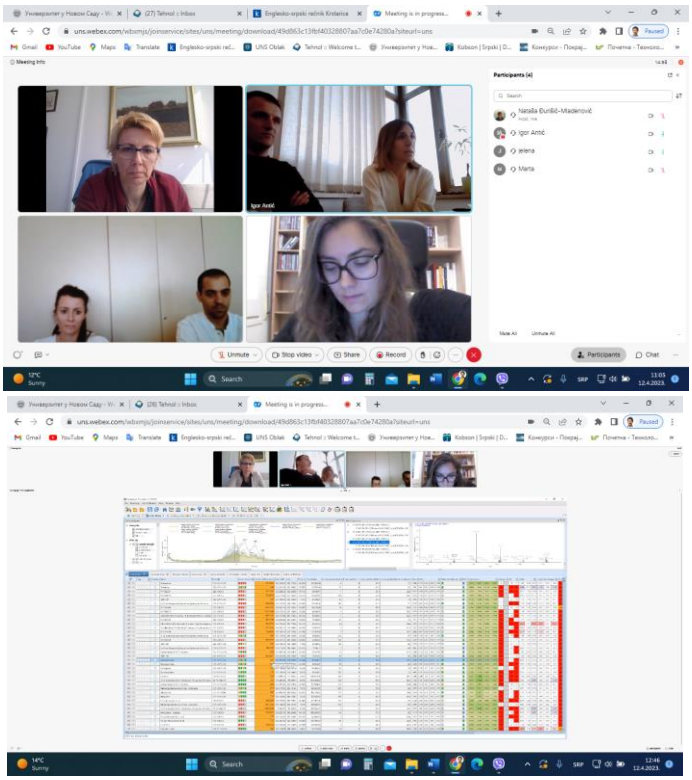
The draft program of the Training was discussed and agreed during an online meeting held on February 26, 2023, atended by the TFNS members from the Lab for Chromatographic Analysis and the members of the CSIC team. During the meeting it was decided to take the 4th onsite training session as an opportunity to learn more on data processing by dedicated software such as Compound Discoverer (Thermo Fisher) using the high-resolution mass spectral data obtained during the analysis of real surface water samples.

Before the agreed onsite training, an online training session was held on April 12, 2023, to discuss additionally some of the tools of the Compound Discoverer Software necessary for data processing. During that online training session, Dr. Marta Llorca, a member of the CSIC team, explained in detail the selection of software available workflows, the setting of data processing parameters in the software, the identification of compounds using MS/MS libraries, the search of online chemical databases, the use of available statistical tools for the interpretation of the obtained results, etc. The attendees were 5 members of the TFNS team from the Lab for Chromatographic Analysis: Dr. Jelena Živančev, Dr. Igor Antić, Dr. Maja Buljovčić, Dušan Rakić, PhD student, and Prof. Nataša Đurišić-Mladenović.

As the TFNS members were already trained for the preparation and analysis of water samples in accordance with the methods and protocols developed in CSIC during the 2nd TwiNSol-CECs

Training (CSIC, Barcelona, November 21-25, 2022), during this latest visit to CSIC, they practiced the gained knowledge preparing a large series of surface water samples, and then learn more analyzing the obtained extracts for the CECs presence. Preparation of surface water samples was based on different solid-phase extraction protocols in order to isolate as wide a range of CECs with different physicochemical properties as possible. Afterwards the analysis of the obtained extracts for the presence of per- and polyfluoroalkyl substances (PFSA) and pharmaceutically active compounds (PhACs) was performed; target and suspect screening analysis of the water extracts were performed by HPLC-HRMS (Q-Exactive). Serbian and Spanish colleagues jointly set the chromatographic and instrumental parameters for the start of the analysis. Finally, the processing of the obtained results was done with a dedicated software tool - Compound Discoverer Software for suspect screening. In this way, the 4th Training represented a training session together with joint research work.

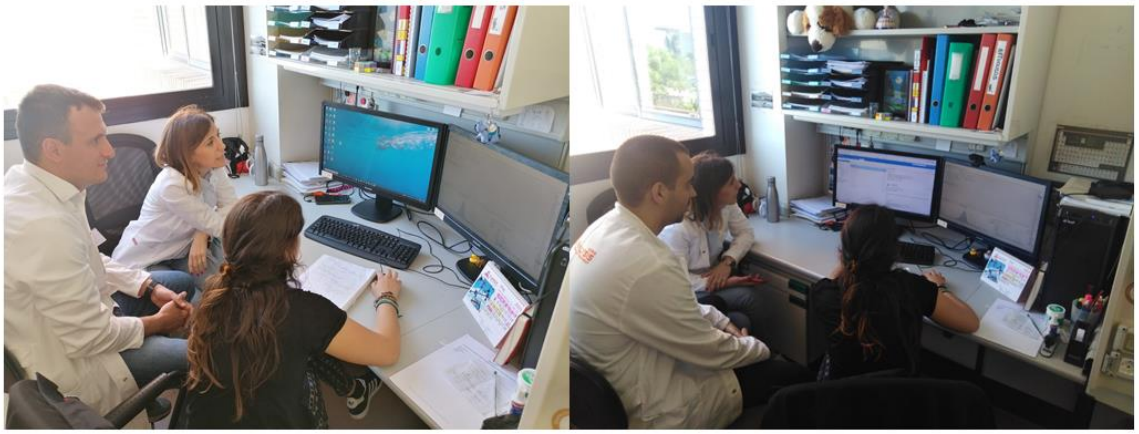
During the last day of the visit, the conceptualization of potential joint articles for submission to international journals, the foreseen short-term scientific exchanges (STSEs), and possible topics and scientific activities in the upcoming period of the TwiNSol-CECs project were discussed.



Online training on selection of Compound Discoverer software available workflows held by Dr. Marta Llorca to TwiNSol-CECs members from the TFNS Laboratory for Chromatographic Analysis on April 12, 2023, as a preparatory session for the subsequent 4th TwiNSol-CECs Training

Visit of TFNS team members to CSIC, IDAEA, Barcelona, during 4th onsite TwiNSol-CECs Training

Preparation of large series of surface water samples for subsequent targeted and suspect screening analysis of PFSAs and PhACs at CSIC, IDAEA, Barcelona



Data processing by Xcalibur software and their analysis for target screening of PhACs and PFASs at CSIC, IDAEA, Barcelona

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organized at Spanish National Research Council, Institute of Environmental Assessment and Water Research (CSIC), Spain,

within the TwiNSol-CECs project (101059867)

08-12 May 2023

PROGRAM

08.05.2023.

Evaluation water sample preparation based on homemade cartridges

09.05.2023.

Evaluation water sample preparation based on commercial single bed cartridges

10.05.2023.

Target screening analysis of PFAS/PhACs in water extracts and data processing

11.05.2023.

Suspect screening analysis of PFAS/PhACs in water extracts and data processing by Compound Discoverer Software

12.05.2023.

Analysis of data collected, discussion on the upcoming STSEs and future analytical challenges

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