Project Deliverable 3.3: Mid-term report on performed trainings

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Abbreviations

CECs	Contaminants of emerging concern
CFD	Computational fluid dynamics
CSIC	Institute of Environmental Assessment and Water Research of the Spanish National Research Council
EGD	European Green Deal
ERA	European Research Area
GA	Grant Agreement
GC	Gas chromatography
GC/MS	Gas chromatography-mass spectrometry
IDAEA	Institute of Environmental Assessment and Water Research
IRIS	Innovation Research and Impact Strategy Office
LC	Liquid chromatography
MPs	Microplastics
MS	Mass spectrometry
PA	Polyamide
PC	Polycarbonate
PCA	Principal component analysis
PE	Polyethylene
PET	Polyethylene terephthalate
PFSA	Per- and polyfluoroalkyl substances
PhACs	Pharmaceutically active compounds
PMMA	Polymethyl methacrylate
PP	Polypropylene
PS	Polystyrene
PST	Project Steering Team
PVC	Polyvinyl chloride
Py-GC/MS	Pyrolysis gas chromatography-mass spectrometry
RMAU	Research management and administration unit
STSEs	Short-term scientific exchanges
TFNS	Faculty of Technology Novi Sad
UNL	NOVA School of Science and Technology
WP	Work Package

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1. Executive summary

This deliverable brings overview of the performed trainings of researchers from University of Novi Sad, Faculty of Technology Novi Sad (TFNS) conducted in the first 15 months of the TwiNSol-CECs project within Work Package (WP) 3 that is dedicated to the reinforcement of the knowledge and skills of TFNS researchers on various aspects of the CECs research. The document gives background information on the planned reinforcement activities in the Introduction section, followed by description of upgrade of the TFNS equipment for widening the scope of the CECs research and on the performed onsite and online trainings given by the researchers from the partner institutions, Institute of Environmental Assessment and Water Research of the Spanish National Research Council (CSIC) and Nova University of Lisbon, NOVA School of Science and Technology (UNL). The trainings have been organized onsite either at TFNS, or the partner institutions, CSIC and UNL, and online. So far, 5 onsite trainings were organized from the start of WP3 in the third project month (October 2022): 2 trainings at CSIC, 1 training at UNL, and 2 at TFNS. Three online training-lectures were held (1 by CSIC and 2 by UNL researchers).

The deliverable D3.3 is the public document, and it is based on continuously prepared reports on each training session organized in the first 15 project months, which have been published at the project website; these reports are appropriately linked (cited) throughout this document. In the Annexes of D3.3, the published reports on the upgrade of the equipment and the program of each onsite training session are presented.

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2. Introduction

In order to step up the excellence of the TFNS resources in the field of the environmental protection research related to advanced analytics and innovative removal technologies for contaminants of emerging concern (CECs), the reinforcement of the TFNS research profiles, materials and human capacities, is foreseen as necessary step to be performed within the TwiNSol-CECs project. The reinforcement is expected to enable gaining of knowledge and skills of the TFNS researchers necessary to tackle the challenges related to CECs, which will influence positively the level of the TFNS integration in the EU networks of excellence, also making the region of Western Balkans more visible within the European Research Area (ERA). This corresponds to the general goal of the project as it targets the harmonization of advanced research and innovation efforts important for the overall faster and sustainable transition of whole Europe foreseen by European Green Deal (EGD) towards zero-pollution, toxic free environment. Enhancement of scientific competences and raising the research profiles of TFNS (senior and early-stage) researchers are planned to be realized by intensive networking with the EU project partners, CSIC and UNL, through performing different joint activities, which are gathered within WP3 - Reinforcing research knowledge and skills of TFNS.

Online and onsite trainings are part of these WP3 activities foreseen as an events of the knowledge- and skill- transfer from CSIC and UNL to the TFNS researchers (both senior and early-stage researchers (ESRs), including PhD students) in domain of the CECs research or on complementary issues important for multidisciplinary approaches in large international research consortia. The training activities are gathered under the Task 3.2 of WP3, which is divided into several subtasks:

Subtask 3.2.1 - Meetings for preparation of the trainings

Subtask 3.2.2 - Organization of the onsite trainings at TFNS

Subtask 3.2.3 - Organization of practical trainings at CSIC and UNL

According to Annex I of Grant Agreement (GA), it was planned to cover different topics in domain of CECs analysis during the onsite trainings at TFNS by CSIC researchers, such as:

- sample preparation and targeted analysis of main group of contaminants of emerging concern in complex samples,
- introduction to suspected screening and non-target analysis by LC and GC coupled to HRMS,
- suspected screening of relevant CECs groups such as micro- and nanoplastics,
- environmental and human health relevancy of CECs determination in water, environmental and food samples,
- introduction to biomonitoring of CECs.

Some of the topics that have been planned originally to be covered by UNL trainers during the onsite trainings at TFNS are:

- adsorption and membrane processes for the removal of organic contaminants from water,
- UV and solar radiation-based processes for CECs degradation,
- linking sustainable development principles and wastewater treatment processes,
- process monitoring, automation, and advanced control,

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- data acquisition and data analysis (including machine learning techniques, when appropriate).

For the onsite trainings at CSIC and UNL, the fixed amount of budget ("grant") is planned per trainee to cover the costs of travel and stay, so it is planned that Committee for Trainings' Grant Approval will be in charge of the trainees' selection based on their motivation letters and CVs (i.e. the main research field). In total, 5 "grants" are planned for the trainings at CSIC and 8 at UNL.

The online trainings are planned to be held as sessions supporting the corresponding onsite trainings and whenever the transfer of knowledge is necessary for enabling continuous research at TFNS.

Additionally, upgrading of the existing advanced analytical instruments at TFNS is planned by GA, enabling the broadening of the CECs-related research at TFNS:

a) installation of a special software with integrated set of MS libraries, for processing of HRMS data is planned, allowing suspect screening besides the already proven target analysis at TFNS,

b) installation of pyrolitic unit on the existing GC/MS will enable additional analysis towards characterization of solid particles, including qualitative analysis of microplastics in water samples, and of various biomaterials (e.g. biochar or other biomass-based products, which are planned to be studies as a "green" adsorbents for the CECs removal from water in WP4),

c) upgrade of the existing membrane systems that enables improvement of the TFNS technical abilities to conduct high-pressure driven processes such as nanofiltration of water samples for removal of CECs.

A part of the training sessions is planned to cover the work with the upgraded equipment at TFNS.

It is expected that reinforced human and material TFNS resources will have an ultimate impact on the improved excellence capacities and resources of TFNS, as well as of the Western Balkans region, enabling to narrow the apparent research and innovation gap within Europe. The networking of TFNS with CSIC and UNL, including the training sessions, will boost the TFNS researchers' knowledge and skills to perform studies beyond the state-of-the-art, bringing important new information for dealing with the problems induced by CECs' occurrence in the environment. These activities will bridge the existing territory gaps in the capacities for environmental and sustainable research throughout Europe.

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3. Upgrade of TFNS material resources for advancing the research on CECs

The upgrade of the existing material capacities at TFNS for the advanced analytics and membrane processes for CECs in water started from the very beginning of the project in order to prepare the equipment for the training sessions on time taking into account the expected very long procurement procedures. The upgrades prolonged the life of the equipment and widened the scope of its application, including the advanced and innovative approaches in the analytics of organic micropollutants and their removal from water.

The installation of planned upgrades is documented in the reports published on the project website after the initial commissioning and training with service engineers of the distributors:

a) In accordance with the work plan of TwiNSol-CECs project, a dedicated software for high resolution mass spectrometric spectra processing (Thermo Scientific™ Compound Discoverer™) was procured for broadening the range of the CECs analysis at TFNS towards the wide-range UHPLC-HRMS screening approach. To support the efficient use of the software, a new PC of high performance (Figure 1) were purchased for the Laboratory for Chromatographic Analysis at TFNS, following the Compound Discoverer™ instructions for the optimal hardware support. The software was successfully installed by an authorized service engineer of the Thermo Scientific distributor in Serbia, who also provided a detailed introductory training (Figure 2). All details on this upgrade are given in the report published on the project website[1], which is also included in Annex I of this document.

Figure 1. *The upgrade for the CECs analysis at TFNS: the Compound Discoverer Thermo Scientific software (box with the provided USB containing all the necessary files for the successful installation) and the computer with advanced performances to support the efficient use of the software*

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[1] https://twinsol-cecs.com/images/documents/r3_2-instalation-of-compound-discoverer_jan_2023.pdf

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b) In accordance with the work plan of the TwiNSol-CECs project, pyrolytic unit *Pyrola® 2000* was procured with an aim to upgrade an existing gas chromatography-mass spectrometry (GC/MS) instrument, enabling broadening the range of compounds of emerging concern that can be analyzed at TFNS towards microplastics (MPs) qualitative determination. Upon receiving the pyrolyzer at the Lab, the installation and the initial training session were performed by an authorized service engineer of the company PYROLab (Lund, Sweden) and an authorized service engineer of the Serbian distributor, DSP Chromatography d.o.o. (Figures 2 and 3). Further details on this upgrade are available in the report published on the project website[2], which is also included in Annex I of this document.

Figure 2. Pyrola® 2000 pyrolyzer and its installation on GC/MS at the Lab for Chromatographic Analysis at TFNS by an authorized service engineers of the company PYROLab (Lund, Sweden) and the Serbian distributor DSP Chromatography d.o.o. (Belgrade, Serbia)

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[2] https://twinsol-cecs.com/images/documents/r32_report-on-pyrola-2000_jan-2023_final.pdf

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Figure 3. *Introductory training on Pyrola 2000 for researchers from the TFNS Lab for Chromatographic Analysis provided by Helena Jönsson, an authorized service engineer of the company PYROLab (Lund, Sweden), at Blue Hall of TFNS*
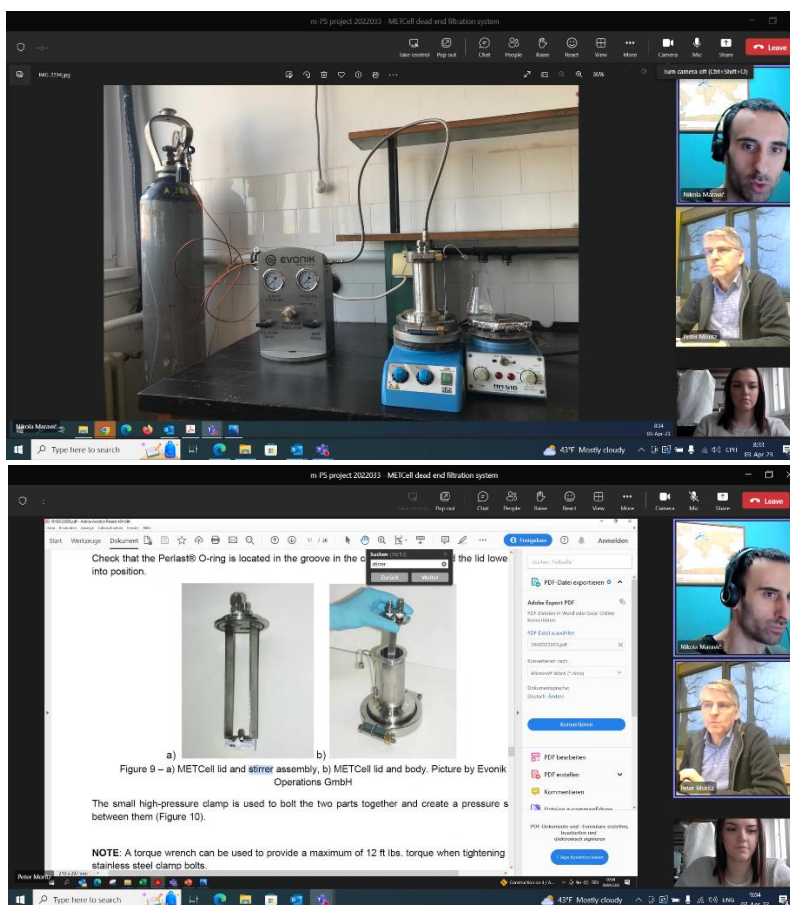
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c) Upgrade of the existing membrane systems at TFNS was planned within the TwiNSol-CECs project to expend the research on membrane separation towards nanofiltration for CECs removal from water. The upgrade has been agreed in accordance with the suggestion of Prof. Joao Crespo, a leading investigator from the project partner institution UNL, given at the very beginning of the project during the online meetings. Prof. Crespo suggested that upgrade of the existing equipment of TFNS would enable improvement of the TFNS technical abilities to conduct high-pressure driven processes such as reverse osmosis or nanofiltration of water samples, also harmonized with the research capacities at UNL. The METcell® was successfully installed at TFNS (Figures 4 and 5) by two members of nanofiltration research within the TFNS project team, Dr. Nikola Maravić and Jelena Šurlan, PhD student, under the supervision of Peter Moritz, Managing Director of m-PS modular process solutions (Allschwil, Switzerland). All details on this upgrade are given in the report published on the project website[3], which is included in Annex I of this document.

Figure 4. Setting up METcell® dead-end filtration unit in TFNS laboratory

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[3] https://twinsol-cecs.com/images/documents/r3_3_report_on_metcell_march_2023.pdf

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Figure 5. Online training session with Peter Moritz from m-PS Modular Process Solutions (Switzerland)

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4. Trainings

The initial discussion of the project onsite trainings started with the very beginning of the project by email correspondence and the online meetings prior the kick-off meeting held at TFNS on October 19, 2022. It was decided that theoretical trainings held at TFNS will be organized for the whole project team, while practical sessions will be attended with those project team members, whose research interest coincides with the topics covered by the training program.

The first onsite training at TFNS was agreed by email correspondence, and it was organized in days before the kick-off meeting, focusing on CECs and the challenges in front of their surveillance in the environment. The intention was to have multiple events in the week when kick-off meeting was scheduled.

Agreement of the following onsite trainings at CSIC and UNL was made during the kick-off meeting at TFNS on October 19, 2022, when it was decided to organize one training at CSIC and one at UNL in the first 3 months of WP3, covering the introduction to the equipment and the achievements of the hosting researchers, transferring the relevant knowledge on the research of interest for the TwiNSol-CECs project: the advanced analytics for the CECs surveillance in water (CSIC) and membrane separation technologies (UNL). In accordance with the working schedule of the hosting researchers and the capacities of their laboratories, number of visiting trainees and the dates were agreed by email correspondence following the kick-off meeting.

In order to follow the original idea from the project description in GA, the Committee for Trainings' Grant Approval was established during the kick-off meeting, consisting of Dr. Marinella Farre, CSIC, Prof. Joao Crespo, UNL, and Prof. Biljana Pajin, TFNS. They have been in charge to arrange distribution of the grants to the trainees based on the training's main topics and the research interest of the team members in accordance to overall project interest to level up the competences and be prepared for the project research. Ten TFNS researchers, including two PhD students, from the TwiNSol-CECs project team, whose research interests coincide with the TwiNSol-CECs research topics, prepared motivational letters explaining why they would like to attend trainings at CSIC and UNL, and what they expect from these trainings with expected outcomes on their career.

All the trainings were announced on the project website and the social media profiles.

The attendance lists for all trainings at TFNS are signed by the participants. All training events, both online and on site, were GDPR compliant.

4.1. Trainings by CSIC

The **1st TwiNSol-CECs Training was organized at TFNS** as a two-day event on **October 17-18, 2022**. The Course is organized through lectures of the CSIC researchers with the aim of transferring the knowledge on various aspects of CECs analysis to the TFNS team members (Figure 6). CSIC team members led by Dr. Marinella Farre, CSIC Project Manager, with prestigious knowledge and expertise

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in the field of CECs analysis, presented the latest trends related to sampling, sample preparation techniques and sample preservation, extraction of CECs from different types (liquid and solid) samples and targeted analysis of CECs belonging to different chemical classes. The program of the 1st onsite TwiNSol-CECs training is included in the Annex II, while more details on the training are available in the report published on the project website[4]. The following CSIC researchers visited TFNS and took a part in the training besides Dr. Farre: Dr. Sandra Perez, Dr. Marta Llorca, Dr. Nicola Montemurro, and Olga Gomez (Figure 7).

Twelve trainees from TFNS project team participated in the Training, verifying the attendance with signatures in the Attendance list. All of them, as well as the trainers, were awarded certificates of participation.

In parallel to the training, working meetings of PST were organized at TFNS, where Dr. Farre and Dr. Lorca participated in line with the program of the training.

Figure 6. Some of the lectures during the 1st TwiNSol-CECs training: Dr. Sandra Perez (left) and Dr. Marinella Farre (right)

Figure 7. CSIC team at TFNS for 1st onsite TwiNSol-CECs training, 17-18 October 2022

Before the 2nd onsite TwiNSol-CECs training planned to be organized by CSIC, the **online meeting** of the selected members of the TFNS and the CSIC teams was held on **November 4, 2022**. The invitation was sent by Dr. Marinella Farre, who also led the meeting. This meeting was dedicated to the

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[4] https://twinsol-cecs.com/images/documents/r3_2_1st_training_tfns-17-18oct2022.pdf

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preparation for the upcoming 2nd onsite training when it was agreed to be held between 21-25 November 2022 at Institute of Environmental Assessment and Water Research (IDAEA) of CSIC, Barcelona. The program of the Training was also discussed and agreed. Afterwards, the principles of the water samples were presented by Dr. Marinella Farre and Dr. Marta Llorca as an introductory lecture on the practical sessions to be held on site during the 2nd training.

The 2nd onsite TwiNSol-CECs Training was organized as a five-day event **on November 21-25, 2022, at IDAEA - CSIC.** It was attended by two representatives of TFNS team members: Dr. Jelena Živančev and Dr. Igor Antić (Figure 8), who both have significant experience in the application of various MS detection-based analytical techniques; in this way, they could easily accept the advanced knowledge in short time frame of the training, and transfer it to other researchers at TFNS, while also applying it for the project research activities.

Agenda of the 2nd TwiNSol-CECs training consisted of practical lessons and necessary work within different, consecutive phases of the CECs screening methods for analysis of per- and polyfluoroalkyl substances (PFSA) and pharmaceutically active compounds (PhACs). The presented methods are those previously developed and valorized by CSIC researchers involved in TwiNSol-CECs project. These methods have been used in CSIC labs for determination of CECs occurrence in different samples, with the results published in highly ranked international journals. Before starting the demonstration of high-resolution mass spectrometric analysis, Dr. Llorca gave a theoretical introduction about HPLC-HRMS technique installed at IDAEA for the CECs wide-scope analysis. Training continued with targeted and suspect screening analysis of PhACs in water extracts, where the role of moderator was played by Olga Gómez. Introduction to data processing and analysis by a dedicated software tool such as Compound Discoverer Software was delivered by Dr. Farre, Dr. Pérez and Dr. Montemurro. Details on the 2nd onsite training are available in the report published on the project website[5].

One more training at CSIC for TFNS researchers with background in chromatographic and MS analytics was organized in the period **May 08-12, 2023. It was the 4th onsite TwiNSol-CECs training** in a row, including the 3rd one organized previously at UNL. The 4th training was one-week visit of three researchers from TFNS, Dr. Jelena Živančev, Dr. Igor Antić, and Dušan Rakić, PhD student, at CSIC (Figure 9). The whole project team from CSIC was included in the training under the leadership of Dr. Marinella Farre. The draft program of the Training was discussed and agreed during an **online meeting held on February 26, 2023**. It was decided to take the 4th onsite training session as an opportunity to learn more on HRMS data processing by dedicated software such as Compound Discoverer (Thermo Scientific) installed recently at TFNS (see Section 3) using the HRMS spectra of water samples. Before the 4th 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 at TFNS; the attendees were 5 members of the TFNS team: Dr. Jelena Živančev, Dr. Igor Antić, Dr. Maja Buljovčić, Dušan Rakić, PhD student, and Prof. Nataša Đurišić-Mladenović.

During the 4th training, TFNS researchers practiced the gained knowledge on preparing water samples, and then learn more analyzing the CECs presence in water samples by HRMS. Finally, the processing of the obtained results was done with a dedicated software tool - Compound Discoverer Software for

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[5] https://twinsol-cecs.com/images/documents/r3_2-2nd_onsite_trening-csic-21-25nov2022.pdf

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suspect screening. During the last day of the visit, the conceptualization of joint research, 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. More details on this training are available in the report published on the project website[6], while the program is presented in Annex I.
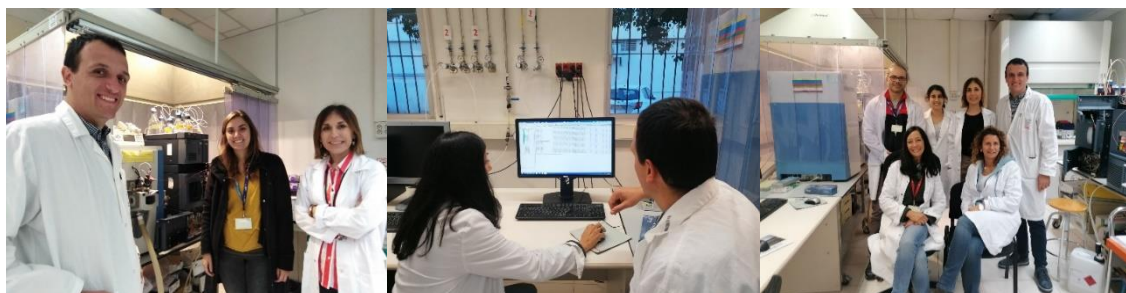
Figure 8. Dr. Živančev and Dr. Antić at IDAEA, CSIC, during the 2nd onsite TwiNSol-CECs training, November 21-25, 2022

Figure 9. Dr. Živančev, Dr. Antić, and Dušan Rakić, PhD student, at IDAEA - CSIC during the 4th onsite TwiNSol-CECs training

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[6] https://twinsol-cecs.com/images/documents/r3_2-4th_onsite_training-csic-8-12may2023.pdf

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4.2. Trainings by UNL

The 3ʳᵈ TwiNSol-CECs training was organized at UNL by Prof. Joao Crespo in the period **December 12-16, 2022**. It was an event dedicated to intensive transfer of advanced knowledge and best practice of UNL staff to representatives of TFNS, two senior researches Prof. Zita Šereš and Prof. Nataša Đurišić-Mladenović, and one early-stage research Dr. Nikola Maravić. Every day of the training was dedicated to subjects of importance either for the joint research at TwiNSol-CECs (within WP4) or for creation of the research management and administration unit (RMAU, WP5); the part of this training related to research skills is a subject of this deliverable, while training on an institutional practice in research management is a subject of deliverable D5.1. All the meetings within the 3ʳᵈ TwiNSol-CECs training enabled for TFNS team members to be more familiar with advanced research and equipment, as well as institutional management and administration efforts at UNL, that have contributed to placing UNL at high-ranking positions within ERA and among European higher education institutions. The team from TFNS participated in laboratory training on the dead-end membrane filtration METCell device and in a complete laboratory exercise on a cross-flow Osmonicsinstallation; other training sessions considered computational tools for support to membrane processes, principals of the advanced oxidation combined with membrane processes, nanofiltration combined with low pressure ultraviolet photolysis (Figure 10). The researchers from the TwiNSol-CECs team coming from UNL, involved in this training session, besides Prof. Crespo, who created the training program as presented in the Annex II, were Dr. Vanessa Pereira, Dr. Clara Brazinha, Dr. Claudia Galinha, and Dr. Sylwin Pawlowski.

Figure 10. TFNS researchers at laboratories of the NOVA School of Science and Technology, UNL

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Figure 11. Presentation of pressure driven membrane processes and reverse electrodialysis by Dr. Clara Brazinha and Prof. Joao Crespo during the 3rd TwiNSol-CECs training at UNL

Figure 12. Detail from the training held at the UNL Institute of Experimental Biology and Technology (iBET) by Dr. Vanessa Pereira

Furthermore, Prof. Joao Crespo, a leader of the project team from UNL created a series of training sessions dedicated to the different topics within the domain of membrane separation processes, starting from the basics of these processes, their application for the removal of organic contaminants from water, process monitoring, automation and advanced control, data acquisition and data analysis. The series of trainings was named "Membrane Separation Technologies in the Spotlight"; the integral report on all the training sessions under this title is available at the project website[7]. Membrane separation technology could be regarded as the one of the main research domains of TwiNSol-CECs project, besides the advanced analytics on Contaminants of Emerging Concern (CECs) and the application of biomaterials for CECs removal.

The first two lectures were held online by Prof. Joao Crespo and Dr. Vanessa Pereira, followed by the 2-day training at TFNS – the 5th onsite TwiNSol-CECs training with two visiting researchers from UNL, Dr. Claudia Brayinha and Dr. Sylwin Pawlowski, who gave both theoretical and practical sessions.

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[7] https://twinsol-cecs.com/images/documents/r3_2-5th_onsite_training-tfns-26-27_september2023_final.pdf

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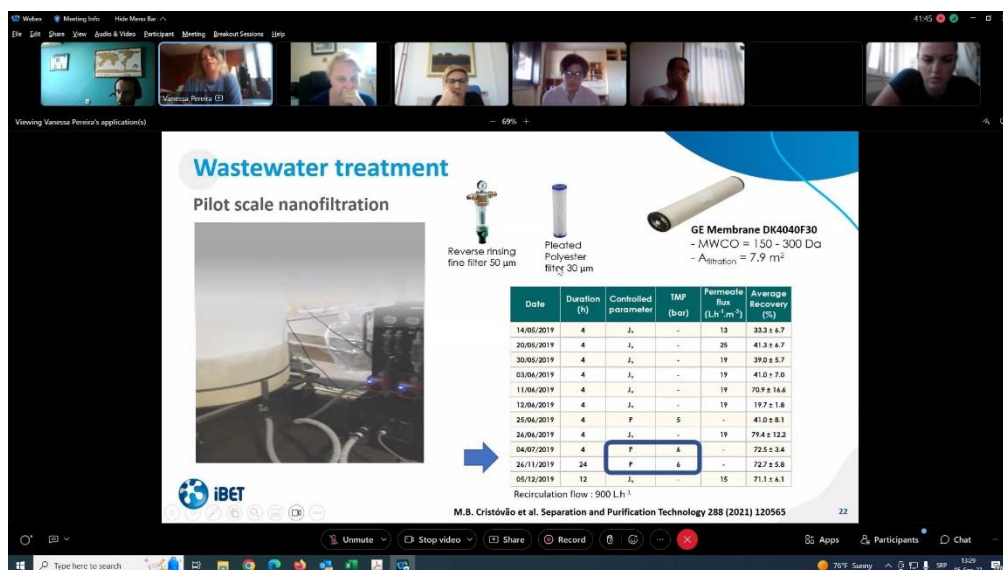
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The opening **online lecture** within the series on membrane processes was held by Prof. Joao Crespo on **August 25, 2023**, 13.00 – 14.10 h CET under the title "Principles of Pressure Driven Membrane Processes". In his lecture, Prof. Joao Crespo has presented main principles regarding pressure driven processes in a time frame of 50 minutes. The participants had an opportunity to hear more about different techniques of managing membrane separation processes. Furthermore, specific problems and solutions in the area of membrane structure, membrane permeance and membrane flux decay were addressed and discussed (Figure 13); industrial scale application and technology were discussed with a presentation of large-scale membrane reactors. At the end of a lecture, Prof. Joao Crespo raised most important questions to be answered in terms of successful application of pressure driven membrane processes. Afterwards, discussion section was opened, and several participants asked questions and gave comments. Discussion section lasted for 20 minutes. The online lecture was recorded and published on TwiNSol-CECs YouTube channel[8].

Figure 13. Printscreen during the online lecture of Prof. Joao Crespo on August 25, 2023

The second **online lecture** within the series "Membrane Separation Technologies in Spotlight" entitled "Principles of Pressure Driven Membrane Processes" was held by Dr. Vanessa Pereira from iBET, UNL, on **September 5, 2023**, 13.00 – 14.10 h CET. In her 45 min presentation Dr. Vanessa Pereira highlighted modern problems with surface water reuse and complexity of the applied treatments (Figure 14). Furthermore, a detailed insight into the membrane processes coupled with different non-membrane treatments to meet specific qualitative demands for water reuse was given. Specific attention was paid to the UV light treatment of both permeate and retentate obtained in nanofiltration of surface water in order to remove/degrade different pharmaceuticals. Dr. Pereira also presented the latest results of the study in which she was involved within the field of pharmaceutics removal from water samples. After the presentation, 25 minutes of discussion took place. Several researchers engaged in discussion with their questions and comments of the presented material.

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[8] https://www.youtube.com/watch?v=-a0aaP78pc4&t=1620s

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Figure 14. *One of the slides during the presentation of Dr. Vanessa Pereira on September 05, 2023*

Both online lectures were moderated by Dr. Nikola Maravić, the project communication coordinator and a member of the membrane technology team from TFNS, followed by the welcome word of Prof. Nataša Đurišić-Mladenović, presenting briefly the importance of the trainings by the EU partners and of the membrane processes for the TwiNSol-CECs project. Subsequently, Prof. Zita Šereš, head of the membrane technology group from TFNS, introduced the UNL lecturer, highlighting the most important parts from their biographies.

The **5th onsite TwiNSol-CECs training** "Computational methods as a support for membrane based separation technologies" was organized as a two-day event on **September 26-27, 2023,** at TFNS. The aim of the Training was to transfer specific knowledge from the UNL researchers, which could be regarded as one of the EU top leading research institution within the domain of membrane separation processes, to TFNS researchers and others interested in membrane processes coming from different institutions. Dr. Claudia Galinha and Dr. Sylwin Pawlowski, from UNL, with prestigious knowledge and expertise in the field of membrane separation processes, particularly in electrospinning, 3D printing, computational fluid dynamics, 2D fluorescence and PCA analysis, held a series of lessons on the topic. The program of the training is attached to the report. The full report on the 5th TwiNSol-CECs training is available at the project website[9]. The training was organized as a combination of theoretical sessions on the first day and practical lessons in a computer room at TFNS during the second day (Figure 15).
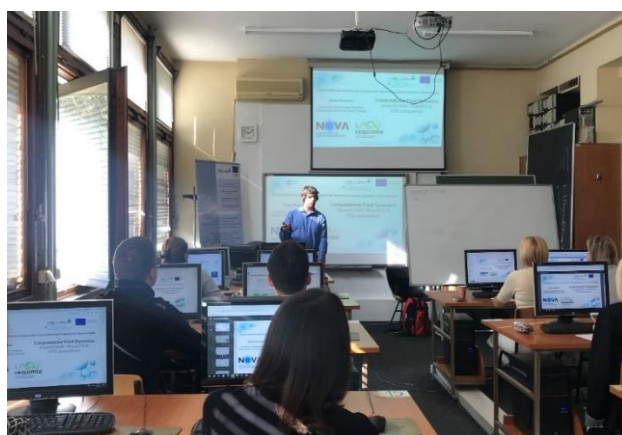
Apart of researchers from the TwiNSol-CECs project, several researchers outside of the project team were invited, knowing their research interest in membrane processes, but due to capacity of the computer room, the number of attendees was limited to maximum 20 for the second day.

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[9] https://twinsol-cecs.com/images/documents/r3_2-5th_onsite_training-tfns-26-27_september2023_final.pdf

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a)

b)

Figure 15. *a) Theoretical lessons held by Dr. Sylwin Pawlowski and Dr. Claudia Galinha at TFNS Blue Hall on September 26, 2023*

b) Practical lessons on computational fluid dynamics (CFD) with Dr. Sylwin Pawlowski and Dr. Claudia Galinha in a computer room at TFNS on September 27, 2023

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The list of full public reports of the TwiNSol-CECs trainings used for preparation of this Deliverable 3.3

Thermo Scientific™ Compound Discoverer™ software for wide range screening of CECs by UHPLC-HRMS https://twinsol-cecs.com/images/documents/r3_2-instalation-of-compound-discoverer_jan_2023.pdf

Upgrade of GC/MS with Pyrola® 2000 pyrolyzer for widening the analytical capabilities of TFNS towards determination of microplatics https://twinsol-cecs.com/images/documents/r32_report-on-pyrola-2000_jan-2023_final.pdf

Instalation of a new dead-end system (METcell®) at Faculty of Technology Novi Sad (TFNS) for TwiNSol-CECs research on nanofiltration in CECs removal from water https://twinsol-cecs.com/images/documents/r3_3_report_on_metcell_march_2023.pdf

1st TwiNSol-CECs Training "Sample preparation and targeted analysis of main group of contaminants of emerging concern in complex samples" https://twinsol-cecs.com/images/documents/r3_2_1st_training_tfns-17-18oct2022.pdf

2nd TwiNSol-CECs Training "High-resolution mass spectrometry application in revealing the CECs presence in water https://twinsol-cecs.com/images/documents/r3_2-2nd_onsite_trening-csic-21-25nov2022.pdf

3rd TwiNSol-CECs training "Transfer of knowledge and best practice for TwiNSol-CECs research and strategic activities" NOVA University of Lisbon, Lisbon, Portugal https://twinsol-cecs.com/images/documents/r3_2-3rd_onsite_training-unl-12-16dec2022.pdf

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 https://twinsol-cecs.com/images/documents/r3_2-4th_onsite_training-csic-8-12may2023.pdf

Series of trainings "MEMBRANE SEPARATION TECHNOLOGIES IN THE SPOTLIGHT" University of Novi Sad, Faculty of Technology Novi Sad (TFNS) August – October 2023 https://twinsol-cecs.com/images/documents/r3_2-5th_onsite_training-tfns-26-27_september2023_final.pdf

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Annex I – Full reports on the equipment upgrade during the first reporting period

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REPORT

Thermo Scientific™ Compound Discoverer™ software for wide range screening of CECs by UHPLC-HRMS

In accordance to the work plan of TwiNSol-CECs project, "*Thermo Scientific™ Compound Discoverer™*" software was procured for the needs of broadening the range of UHPLC-HRMS analysis towards the wide-range screening of Contaminants of Emerging Concern (CECs). In fact, *Compound Discoverer™* is a small molecule identification application for high-resolution liquid chromatography (LC) – mass spectrometry (MS) and gas chromatography (GC) Orbitrap data. To support the efficient use of the software, a new PC of high performance with two display monitors were purchased following the *Compound Discoverer™* instructions for the optimal hardware support (Figure 1).

UHPLC-HRMS system existing at TFNS is Thermo Scientific™ Accela Exactive instrument with Orbitrap™ mass spectrometers. This system has been used for target analysis and compound mass confirmation, and even though the HRMS unit produces information-rich data without the dedicated software support they cannot be used for wide-range screening. To overcome of this and other challenges of small-molecule analysis a powerful software is required.

With a comprehensive, integrated set of libraries, databases, statistical analysis and visualization tools linked in customizable workflows, the *Compound Discoverer™* software streamlines unknown identification, determination of real differences between samples, and elucidation of biological pathways. Additionally, the software reveals the highest confidence data obtained on LC and mass spectrometry (MS) instrumentation.

For successful data processing appropriate computer configuration (hardware and software) is required according to the recommendations provided in *Compound Discoverer™* User Guide for LC Studies (Software version 3.3, XCALI-98478 Revision A, November 2021), Figure 2. The User Guide specifies hardware (processor, RAM memory, display monitor resolution, DVD-ROM, USB), software (operating program, Microsoft Offices version, etc.), and system settings requirements for processing computer. The purchased computer configuration satisfies the recommended hardware configuration for enhanced performance.

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Figure 1. *The box with the provided USB containing all the necessary files for the successful installation of the Compound Discoverer software and the computer (hardware and software) together with display monitors*

The software was successfully installed at the TFNS by Dr. Luka Milovanović, an authorized service engineer of the company (Analysis d.o.o., Belgrade), representative of Thermo Scientific™ instruments and software installation in Serbia (Figure 3).

After the software installation, a detailed introductory training was provided by Dr. Luka Milovanović, who demonstrated the main software tools (Figure 4), including:

- Setting the data processing parameters in the software
- Identification of compounds using MS/MS libraries
- Determination of elemental composition using high-resolution full MS isotopes and MS/MS data
- Search online chemical databases
- Gaining confidence in ID with automated MS^n tree search against mzCloud
- Performing the statistics and differential analysis using t-tests, ANOVA, PCA, PLS-DA, volcano plots, box-and-whisker plots, and more
- Viewing trend charts to visualize peak areas, average peak area per group or fractional label incorporation over time, etc.

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Table 1. Hardware and software requirements for the processing computer

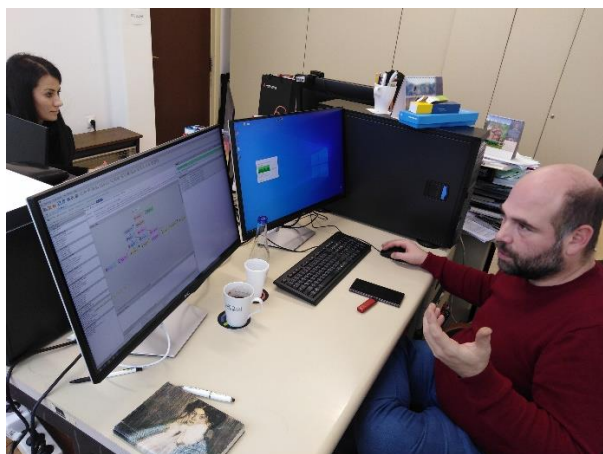| System	Minimum requirements
Hardware	• 3.4 GHz dual-core processor • 16 GB RAM • 500 GB hard drive • DVD-ROM and USB drive • Display monitor resolution of 1920 × 1080
Software	• Microsoft Windows 7 SP1 64-bit operating system or Microsoft Windows 10 64-bit operating system • Microsoft .NET Framework 4.7.2 • Microsoft .NET Core Runtime 2.1.19 • Microsoft Office 2013 • PDF reader
System settings	• To run processing workflows with online mass spectral database searches, the computer must have unblocked access to the mass spectral databases on the Internet. • The computer must have the correct time and date settings and be synchronized with Internet time. • The Region and Language setting for the operating system must be set to English (United States).

Preface

Table 2 lists the recommended hardware configurations for enhanced performance using the Compound Discoverer application.
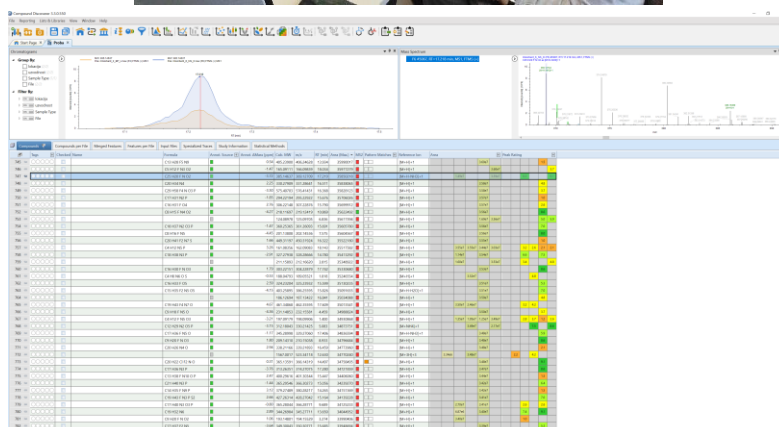
Table 2. Recommended hardware configurations for enhanced performance

System	Recommended configurations
Hardware	• Dual 8-core processor (for example, 2x Intel™ Xeon™ Gold 6134 CPU @ 3.20 GHz) • 64 GB RAM • 1 TB SSD (solid-state disk) hard drive for OS • 2nd 3 TB (conventional disk) hard drive for data storage • DVD-ROM and USB drive • Two 27 in. UHD monitors: Display monitor resolution of 3840 × 2160 pixels

Figure 2. *Specified computer* configuration *(hardware and software) for software installation*

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Figure 3. *Installation of software by authorized service engineer Dr. Luka Milovanović*

Figure 4. *Detailed introductory training on data processing (real sample analysis) on Compound Discoverer software*

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REPORT

Upgrade of GC/MS with Pyrola® 2000 pyrolyzer for widening the analytical capabilities of TFNS towards determination of microplatics

In accordance with the work plan of the TwiNSol-CECs project, "*Pyrola® 2000 pyrolyzer*" was procured with an aim to upgrade an existing gas chromatography-mass spectrometry (GC/MS) instrument and in this way to broaden the range of compounds of emerging concern that can be analyzed at TFNS towards microplastics (MPs) determination. The GC/MS system available at the Lab for Chromatography at TFNS is *Agilent 7890B GC* with *Agilent 5977A MS*. Upon receiving the pyrolyzer at the Lab, the installation and training session were agreed with the Agilent distributor for Serbia (DSP Chromatography d.o.o., Belgrade) and organized at the Lab on Jan 17-18, 2023.

So far, GC/MS has been used for target/screening analysis of deferent volatile and semi-volatile organic compounds (terpenes, persistent organic pollutants, pesticides, phthalic acid esters, etc.). Analysis of MPs in environmental samples represents a significant challenge. Pyrolysis gas chromatography-mass spectrometry (Py-GC/MS) is a common technique used in polymer science including analysis of environmental samples to get quality and quantity information regarding the presence of MPs. Py-GC/MS can be used to identify and quantify commonly used polymers that make MPs, i.e. polyethylene - PE, polypropylene - PP, polystyrene - PS, polyvinyl chloride - PVC, polyamide - PA, polymethyl methacrylate - PMMA, Polycarbonate - PC, and polyethylene terephthalate - PET.

In general, *Pyrola® 2000* pyrolyzer offers opportunities for analysis of non-volatile samples by making them volatile by heating a sample in an inert atmosphere so the large molecules are divided into smaller more volatile fragments. The *Pyrola® 2000* system consists of the process unit, control unit, optic cable, control cable to the processing unit, communication cable, main power cable, and computer with *Pyrola® 2000* software.

The pyrolyzer was successfully installed at TFNS (Figures 1-2) by Helena Jönsson, an authorized service engineer of the company PYROLab (Lund, Sweden) and Mladen Perišić, an authorized service engineer of DSP Chromatography d.o.o. (Belgrade, Serbia).

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Figure 1. Pyrola® 2000 *pyrolyzer (left) and its installation on GC/MS at the Lab for Chromatography at TFNS*
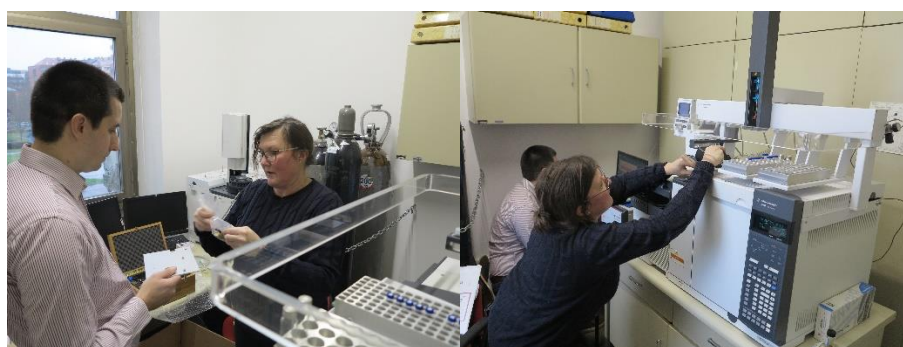
Figure 2. *Installation of* Pyrola® 2000 *pyrolyzer*

After the software installation, a detailed introductory training was provided by Helena Jönsson, who demonstrated the main hardware and software tools (Figure 3), including:

- Detailed explanation of all *Pyrola® 2000* unit
- Connection and disconnection of the *Pyrola® 2000* unit from the GC system
- Description and usage of the software
- Application of different pyrolysis techniques: isothermal desorption, sequential pyrolysis, fractionated pyrolysis, and pyrotomy
- Analysis of real samples
- Maintenance of the *Pyrola® 2000* unit

The upgraded instrument, Py-GC/MS, is labeled with TwiNSol-CECs sticker (Figure 4); further training sessions within TwiNSol-CECs, dealing with MPs analysis by Py-GC/MS are expected to be agreed with CSIC partner.

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Figure 3. *Introductory training on* Pyrola 2000 *for TFNS team members from the Lab for Chromatgraphy provided by Helena Jönsson,* an authorized service engineer of the company PYROLab (Lund, Sweden)

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Figure 4. Pyrola 2000 *process unit installed on the (top of) existing GC/MS instrument at TFNS with the* Pyrola *control unit (on the left) labeled with TwiNSol-CECs sticker*

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REPORT

Installation of a new dead-end system (METcell®) at Faculty of Technology Novi Sad (TFNS) for TwiNSol-CECs research on nanofiltration in CECs removal from water

Upgrade of the existing membrane systems at TFNS was planned within the TwiNSol-CECs project and the Work Package (WP) 3 - Reinforcing research knowledge and skills of TFNS, but also to be capable to perform the research planned within WP4. The upgrade has been agreed in accordance with the suggestion of Prof. Joao Crespo, a leading investigator from the project partner institution, NOVA University of Lisbon (UNL), given in the very beginning of the project during the online meetings. Prof. Crespo suggested that upgrade of the existing equipment of TFNS with similar or the same unit as the one existing at UNL would enable improvement of the TFNS technical abilities to conduct high-pressure driven processes such as reverse osmosis or nanofiltration of water samples, also harmonized with the research capacities at UNL. The chance for TFNS representatives to learn more about METcell® dead-end system and its applicability in CECs research was during the visit to UNL during December 2023, when training on putting the device into operation was conducted on the existing unit at UNL.

The METcell® set of equipment was designed by EVONIK Company to be an easy entry point for scoping separations process development at lab scale, using flat sheet membranes. Upon receiving the METcell® at the Lab, the installation and training session were agreed with the official distributor for Europe (m-PS Modular Process Solutions, Switzerland) and organized online on April 3rd, 2023.

The METcell® is a 316 stainless steel high-pressure stirred cell that is capable of performing a wide range of membrane separations. It has a maximum working pressure of 69 bar and is suitable for reverse osmosis and nanofiltration separations using aqueous and non-aqueous solvents. O-ring seals are used to allow high-pressure operation. The METcell® is pressurized using gas from a cylinder (typically using an inert gas such as nitrogen) and with the MET Gas Unit supplied with each METcell®.

Through the application of METcell® dead-end system in lab scale nanofiltration experiments, TFNS will be able to effectively test multiple membrane materials, filtration processing conditions and different size exclusion parameters (membrane pore size, MWCO, etc). METcell® provides easy-to-use design, with easily removable top to charge feed solution, and easily removable base for membrane replacement which allows great reproducibility of tested operating and processing conditions.

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So far, METcell® has been used in state-of-the-art nanofiltration research published in the high rank membrane science journals by multiple authors.
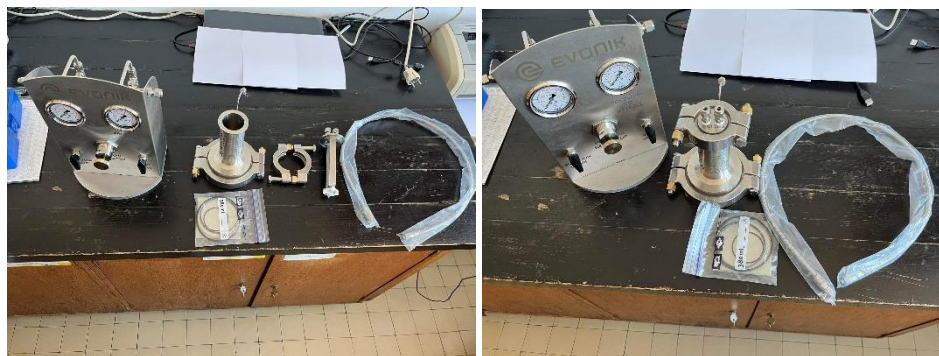
Figure 1. *METcell® dead-end system components*
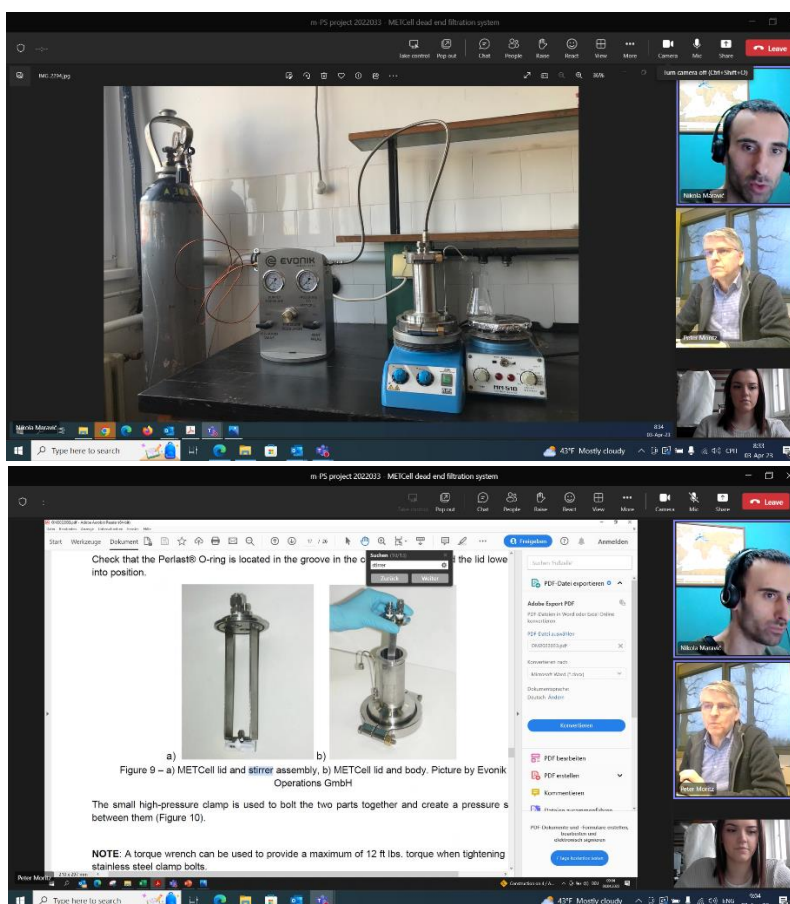
Figure 2. *Online training session with Peter Moritz from m-PS Modular Process Solutions (Switzerland)*

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The METcell® was successfully installed at TFNS (Figures 1-2) by Dr. Nikola Maravić and Jelena Šurlan, PhD student, as a members of nanofiltration research team within TwiNSol-CECs project, under the supervision of Peter Moritz, Managing Director of m-PS modular process solutions (Allschwil, Switzerland).

Figure 3. *Setting up METcell® dead-end filtration unit in TFNS laboratory*

Figure 4. *METcell® dead-end filtration unit installed at the TFNS laboratory labeled with TwiNSol-CECs sticker*

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Annex II – Programs of the onsite TwiNSol-CECs trainings

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1st TwiNSol-CECs Training

"Sample preparation and targeted analysis of main group of contaminants of emerging concern in complex samples"

organized at University of Novi Sad, Faculty of Technology Novi Sad, Serbia

17-18 October 2022

Program

17 Oct 2022		18 Oct 2022	
10.00-11:00	Sampling *Nicola Montemurro*	9.00-10:00	Target analysis of pharmaceutical compounds polar compounds and transformation products *Sandra Pérez*
11:00-11:30	*Coffee break*	10:00-10:30	*Coffee break*
11:30-13:00	Introduction to sample preparation techniques,QA/QC during sampling, sample preservation *Marta Llorca*	10:30-12:00	Target analysis of PFAS and emerging PFAS and other PMOCS *Marta Llorca*
13:30-14:30	*Lunch*	12:00-12:30	*Lunch*
14:30-15:30	Extraction of CEC from liquid samples *Olga Gómez*	13:30-14:30	Target analysis of Anthropogenic particles: Nanomaterials and microplastics *Marinella Farré*
15:30-16:30	Extraction of CEC from solid samples *Nicola Montemurro*	14:30-15:30	Natural toxins *Marinella Farré*

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2nd TwiNSol-CECs Training

"High-resolution mass spectrometry application in revealing the CECs presence in water"

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

21-25 November 2022

PROGRAM

21.11.2022.

09,00-17,00 Extraction of CECs from water samples using homemade cartridges

13,00-14,00 Lunch break

22.11.2022.

09,00-17,00 Extraction of CECs from water samples using commercial single bed cartridges

13,00-14,00 Lunch break

23.11.2022.

09,00-17,00 Target and suspect screening analysis of PFAS in water samples

13,00-14,00 Lunch break

24.11.2022.

09,00-17,00 Target and suspect screening analysis of PhACs in water samples

13,00-14,00 Lunch break

25.11.2022.

09,00-17,00 Introduction to data analysis by Compound Discoverer Software

13,00-14,00 Lunch break

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3ʳᵈ TwiNSol-CECs training
"Transfer of knowledge and best practice for TwiNSol-CECs research and strategic activities"
organized at NOVA University of Lisbon (UNL)
12-16 December 2022

Program

12 December 2022

9,00-12,00 Mafalda Cadima, Operation of MetCell and Osmonics installation

12,00-13,30 Lunch break

13,30-14,30 Cláudia Galinha, Machine learning;

14,30-15,30 Carla Brazinha, Membrane contactors/emulsification;

15,30-16,30 Sylwin Pawlowski, Electromembrane processes and Computational Fluid Dynamics

16,30-17,00 Visit to lab for 3D printing and electrospinning

13 December 2022

9,00-12,00 Working meeting for planning the project activities in 2023 – training and short term scientific exchange (STSE)

12,00-13,30 Lunch break

13,30-17,00 Working meeting for planning the project activities in 2023 – joint research and presentations

14 December 2022

9,00-12,00 Vanessa Pereira, Advanced oxidation combined with membrane processes, Visit to iBET labs on advance oxidation processes and semi-industrial nanofiltration unit

12,00-13,30 Lunch break

13,30-15,00 Maria Rosario Bronze, Naiara Fernandez Hernandez, Visit to iBET Food and Health Division labs

15 December 2022

9,00-12,00 Working session I at Innovation Research and Impact Strategy Office (IRIS) and International office at FCT:

Juliana Monteiro, Executive Director of IRIS, and Marta Cerejo, Head of Intellectual Property & Tech Transfer Department, Introduction to IRIS

Bernardo Hourmat, Pre-award (training) services

12,00-13,30 Lunch break

13,30-17,00 Working session II at IRIS office and International office

Miguel Martins, Nova Research Portal

Marta Cerejo and Pedro Almeida, Knowledge valorization and intellectual assets

16 December 2023

9,00-12,00 Meeting at UNL Rectorate

Elsa Caetano, Catarina Pinto and António Grilo, Presentation of Doctorate School project

12,00-13,30 Lunch break

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4th TwiNSol-CECs Training
"*Target and suspect screening of CECs present in surface water samples*"
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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5th TwiNSol-CECs Training
"Computational methods as a support for membrane based separation technologies"
University of Novi Sad, Faculty of Technology Novi Sad
September 26-27, 2023
Program

September 26, 2023 Tuesday
Blue Hall, 1st floor

10,00-10,30	Registration of participants
10,30-10,35	Welcome speech, Prof. Zita Šereš (TFNS, Novi Sad, Serbia)
10,35-10,45	Membrane processes in TwiNSol-CECs, Prof. Nataša Đurišić-Mladenović (TFNS, Novi Sad, Serbia)
10,45-11,30	2D fluorescence for monitoring and characterization of membranes, Claudia Galinha (NOVA University, Lisbon, Portugal)
11,35-12,20	New techniques for development of membranes and devices: electrospinning and 3d printing, Sylwin Pawlowski, (NOVA University, Lisbon, Portugal)
12,20-12,35	Refreshment and coffee break
12,35-13,20	Data analysis and modeling applied to spectroscopic data, Claudia Galinha (NOVA University, Lisbon, Portugal)
13,20-14,05	Computational Fluid Dynamics – Theoretical introduction, Sylwin Pawlowski, (NOVA University, Lisbon, Portugal)
14,05-15,00	Lunch

September 27, 2023 Wednesday
Computer Lab no.10, 1st floor

09,30-10,15	Computational Fluid Dynamics – BlueCFD, Sylwin Pawlowski, (NOVA University, Lisbon, Portugal)
10,20-11,05	Data analysis (PCA and multivariate regression), Claudia Galinha (NOVA University, Lisbon, Portugal)
11,05-11,15	Pause
11,15-12,00	CFD - meshing, numerical schemes, Sylwin Pawlowski, (NOVA University, Lisbon, Portugal)
12,05-12,50	CFD - RTD simulations, Sylwin Pawlowski, (NOVA University, Lisbon, Portugal)
12,55-14,00	Lunch