March 2024

NORMAN Joint Programme of Activities (JPA 2024)

List of scientific activities organised by the NORMAN network in 2024

We are proud to present the scientific programme which will be promoted by the NORMAN network in 2024.

The *NORMAN Joint Programme of Activities* (JPA) is defined every year by the Steering Committee, after consultation with the membership (General Assembly meeting and e-mail survey).

The final JPA and the associated budget are approved by the Steering Committee, using the following criteria:

- the level of interest of the members (results of the survey);
- the relevance of the research topic to European environmental policies;
- the balance between different sectors / fields of interest;
- the relative value of the proposed in-kind contribution *vs* amount of resources required.

For this JPA the Steering Committee has approved a budget of € 264,500, based on the expected income from membership fees of the Founding and Ordinary members. These resources will be allocated for scientific and coordination activities and regular updating and maintenance of the NORMAN Database System.

The JPA of the NORMAN network is financed by the contributions of its members (membership fees and members' in-kind contributions), always with a view to maximising synergies between research teams in the field of contaminants of emerging concern (CECs) and improving the science-to-policy interface at national, European and international level.

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NORMAN NDS – Maintenance and upgrading

NORMAN Database System (Activity coordinated by EI, slobodnik@ei.sk)

The NORMAN Database System (NDS) is a joint activity of all NORMAN members and at the core of the NORMAN activities, providing data and tools to fulfil its goals and visions. The NDS consists nowadays of 13 integrated databases modules:

1. Suspect List Exchange - https://www.norman-network.com/nds/SLE/
2. Substance Database - https://www.norman-network.com/nds/susdat/
3. Chemical Occurrence Data (EMPODAT) - https://www.norman-network.com/nds/empodat/
4. Ecotoxicology Database - https://www.norman-network.com/nds/ecotox/
5. Digital Sample Freezing Platform (DSFP) - https://norman-data.net/Verification/
6. Substance Factsheets - https://www.norman-network.com/nds/factsheets/
7. MassBank Europe - https://massbank.eu/MassBank/
8. Passive Sampling - https://www.norman-network.com/nds/passive/
9. Antibiotic Resistance Bacteria/Genes - https://www.norman-network.com/nds/bacteria/
10. SARS-CoV-2 in sewage - https://www.norman-network.com/nds/sars_cov_2/
11. Bioassays Monitoring Data - https://www.norman-network.com/nds/bioassays/
12. Indoor Environment - https://www.norman-network.com/nds/indoor/chemicalSearch.php
13. Prioritisation - https://www.norman-network.com/nds/prioritisation/

All NDS modules can be searched either individually or starting from the module 'Search All Databases' (https://www.norman-network.com/nds/common/), where any substance from SusDat can be searched and displayed with all available data for this substance in any of the database modules.

All NDS modules underwent continuous update in 2023 and a NORMAN Database workshop took place in Athens on 26 – 27 October 2023 to discuss strategies for further development of the NDS and to provide a platform for technical discussions among the networks' IT experts.
The EMPODAT database grew from ca. 38 million data entries in 2022 to more than 96 million data in the end of 2023 with monitoring data for 4,453 substances. The data stored in EMPODAT are exchanged with the EC IPCHEM on an annual basis. A novel way of formatting the data for upload into the IPCHEM has been agreed between the NDS Development Team and IPCHEM team in November 2023.
The Data Collection Templates have been upgraded and their format harmonised for surface water, ground water, wastewater, sewage sludge, sediments, biota, soil, antibiotic resistance bacteria/genes (ARB/ARGs) and passive sampling. A significant number of new data were uploaded in the Indoor environment (>177,000) and Passive sampling (>4,200) database. Details about the SLE and DSFP are provided in dedicated sections of the JPA 2024.

The tasks for maintenance of the NDS and its continuous upgrade in 2024 will address:

- Critical consideration of the outcomes of the NORMAN Database Workshop. Development of a roadmap/ strategy for further development of the NDS;
- Development of API portal allowing for automated data sharing with external databases;
- Assigning DOI to all contributed datasets in the NDS;
- Further interlinking of all NDS modules and quality check of all input data (it is envisaged that this task could be supported by an appointed QA/QC Expert Group);
- NDS Chemical Occurrence Data (EMPODAT): maintenance, upgrading and feeding of new data into the database. sharing the data with IPCHEM;
- Cooperation with EEA on gathering data on Antibiotic Resistant Bacteria and Genes (ARB/ARG);
- Development of data mining tools to extract raw data from publications, patents and grey literature and establishment of a workflow for their processing into the 'NORMAN format';
- Implementation of visualisation tools in the NDS as agreed in the NORMAN Database Workshop (in collaboration with WG-1);
- Continuous upgrade, maintenance and curation of SusDat (EI in collaboration with NKUA);
- Close collaboration with the NORMAN-SLE team for the development of an open software/packages/approaches for curation/merging of chemical substances in NORMAN-SLE and NORMAN SusDat (EI in collaboration with LCSB – see next entry);
- Update of Passive Sampling module with new datasets. programming of Passive Sampling – SUSPECT module;
- Upload of new data into the ARBs/ARGs module (JDS4, EMBLAS, The Cruise of Three European Seas, etc.);
- Upgrade of Substance Factsheets module – systematic collection of all data needed for prioritisation and data download functions;
- See following sections for more details on NORMAN-SLE, SusDat, MassBank, DSFP and Bioactivity.

NORMAN Suspect List Exchange (NORMAN-SLE)

NORMAN Suspect List Exchange (Leader: LCSB, Luxembourg emma.schymanski@uni.lu)

The NORMAN Suspect List Exchange (NORMAN-SLE) is an initiative of the 2015 Joint Programme of Activities and is an established central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. The NORMAN-SLE (DOI: 10.1186/s12302-022-00680-6) and the compiled suspect list "NORMAN SusDat" (see next section) are the cornerstone/data basis for all NORMAN Database System (NDS) modules and prioritisation efforts.

Activities in 2024 will focus on expanding the efforts from recent years, including:

- Website maintenance and development;
- Addition of new lists from external contributors when they become available;
- Addition/update of contents in existing lists as required;
- Addition of new lists strategically selected to fill identified knowledge gaps;
- Addition/update of lists to specifically save/register/link transformation product information.;
- Archiving of all datasets on Zenodo (https://zenodo.org/communities/norman-sle);
- Automation of various aspects of the SLE (statistics, curation, etc);
- Deposition of all substances in PubChem;
- Integration of lists into PubChem;
- Provision of merged deposition as input to SusDat to assist in merging new entries (see next entry);
- Continuing development of new strategies to deal with UVCBs;
- Further development of strategies to deal with tentative/unknown/related structures;
- Work together with the NORMAN SusDat team to develop open software/packages/approaches for curation/merging between NORMAN-SLE and NORMAN SusDat;
- Plans for a NORMAN-SLE update publication (new lists, developments since 2022) in ~2025

NORMAN SusDat

NORMAN SusDat maintenance and upgrading (Leader: EI alygizakis@ei.sk / slobodnik@ei.sk)

By the end of 2023, the NORMAN-SLE contained 111 lists. Ten new lists were merged and uploaded into SusDat in 2023, which grew from 106,737 to 120,522 substances. There is a need to collect all supporting data required for suspect screening (cf. separate JPA on DSFP) and prioritisation (cf. separate JPA WG-1) of the new 13,785 substances, which represents a challenge for 2024. Thanks to the significant effort of the NDS Development Team, automated curation tools supported with the manual control resulted in removal of 4,209 duplicate entries based on the name or CAS No. of the substances. There are however, 280 duplicates based on the StdInChIKey, which still need attention and appropriate strategy how to deal with them. A new 'batch conversion of identifiers' feature with a guidance has been made available in SusDat (see new icon!), allowing for seamless conversion among names / CAS. Nos./ StdInChIKey/ NORMAN SusDat ID of any (group of) substances in SusDat. Once NORMAN SusDat IDs are generated, they can be directly used for batch searches, e.g., in EMPODAT or in the prioritisation modules.
Publication: NORMAN-SLE & SusDat leads are aiming for a SusDat publication in 2024.

MassBank Europe and RMassBank

MassBank Europe and RMassBank - Continuous development and upgrade of MassBank Europe and related activities (Emma Schymanski & Anjana Elapavalore (LCSB Luxembourg) in co-operation with Tobias Schulze (UBA Berlin), Steffen Neumann (IPB Halle) and Michael Stravs (Eawag)). Contact: massbank@massbank.eu

- Upload of mass spectra to MassBank. All NORMAN members are welcome to contribute!
- Further maintenance / development of RMassBank, MassBank server platform (e.g. database and applications programming interface, curation of records, import and export of records, standardisation of curation rules)
- Fostering the integration of MassBank with other mass spectral and metadata platforms (e.g. MoNA, PubChem, GNPS, US EPA CompTox, NORMAN SusDat, RforMassSpectrometry, etc.)
- Fostering the discussion with vendors for better integration of vendors' software with MassBank
- Continuing discussions on prioritised compounds missing in MassBank (matches to SLE, priority mixtures etc.)
- Making MassBank more FAIR (e.g. better integration of ontologies, linked to NFDI4chem)
- Integration of MassBank in NFDI4chem as central repository (2020-2025)
- MassBank EU publication – scoping and planning under discussion with key Consortium members. Aiming for publication (or at least submission) in 2024.

NORMAN DSFP

DSFP maintenance and upgrading (Leader: EI alygizakis@ei.sk)

DSFP has been used in a series of sampling campaigns and collaborative trials of NORMAN Association, providing satisfactory results in terms of identifying substances usually overlooked by target monitoring. DSFP is nowadays frequently used in various large-scale monitoring campaigns and acting as a safety-net for the detection of potentially hazardous substances. DSFP has proven to be useful for various activities of the NORMAN network, especially at the prioritisation of CECs and as an early-warning system for chemical risks. The previous JPAs focused on upscaling and improvement of Digital Sample Freezing Platform (DSFP) were implemented successfully establishing a significant infrastructure for NORMAN Association. The purpose of the activities was to bring the prototype to a production-ready facility with improved informatic characteristics (usability, maintainability, scalability, performance and extensibility). The activities allowed the implementation of FAIR principles and the establishment of a well-document API for the automatic retrieval of the occurrence of contaminants in stored collections.

As of September 2023, the platform has been populated with HRMS data of 3,870 unique samples. The samples covered environmental samples: surface water (28.68 %), biota (22.97%), wastewater (24.21%), sediment (3.41%), groundwater (3.49%), soil (1.86%), and other matrices (2.82%) and human biomonitoring (12.56%).

The continuous development of functionalities of DSFP is of importance to expand its use and further enrich the database. Changes that would make DSFP more efficient and that would stimulate the interest of researchers to upload their data and thus increase the collection of the HRMS data remain still a very important objective.

The JPA 2024 aims to maintain and improve the functionalities of DSFP:

- Screening and indexing all collections in DSFP to prepare them for EMPODAT-SUSPECT;
- Incorporating a statistical plugin for the analysis of NTS data (unsupervised methods);
- Applying mixture evaluation using network analysis;
- Making the standardised NTS workflow available to the scientific community using Docker technology. This approach allows the execution of the NTS workflow at a high scale in an isolated virtual environment containing all necessary software and dependencies;
- Standardising the output elements of DSFP using controlled vocabulary for metadata, component lists, and screening outputs;
- Creating API mechanisms for predicting all necessary information for importing new compounds;
- Testing 4D-HRMS data from all vendors and updating the DSFP cookbook;
- Investigating the possibility of integrating DSFP with MassBank and RMassBank;
- Creating guidance documents and videos for DSFP;
- Preparing a manuscript describing the new technologies utilised to upscale DSFP;
- Introducing necessary functionalities to allow the use of DSFP in other fields, such as human biomonitoring;
- Maintaining and supporting current and future users, including connection with PARC and other EU-funded projects of NORMAN members.

NORMAN BioActivity Database

NORMAN BioActivity Database (Leader: KWR Water Research Institute Tessa.Pronk@kwrwater.nl Astrid.Reus@kwrwater.nl. Miina.Yanagihara@kwrwater.nl in collaboration with UBA Peter.VonderOhe@uba.de . EI slobodnik@ei.sk)

Understanding the specific responses of individually tested compounds in bioassays is instrumental to the validation and interpretation of the overall responses of these bioassays to environmental samples or for deriving trigger values. In 2020, the NORMAN network embarked on the development of the BioActivity Database (BADB). This database serves as a repository capable of hosting and making searchable the activity and toxicity data measured in *in vitro* bioassays for individual water-relevant chemicals. Its purpose extends to tasks such as:

- Mixture modelling: Exploring the combined effects of various compounds;
- Bioassay selection: Identifying relevant bioassays for water quality monitoring;
- Chemical prioritisation: Determining which chemicals should be included in monitoring programmes based on their potencies and contribution to observed environmental effects.

A prototype of the interface was delivered in 2021 followed by the development of a first Data Collection Template (DTC) and testing on some datasets. Following an expert group consultation in 2023, the data collection template (metadata, controlled vocabulary for the DCT) and the interface have been improved. The goal was to align the final

product with user expectations regarding comprehensive information while minimising the time and effort required for database population. In addition, further effort has been made to ensure alignment with the metadata from the SciRAP tool (SciRAP - Start).

Following these essential enhancements, the BADB will be ready to receive data from collaborators who have committed to participating in this task during 2024.

The main activity for 2024 will be to first compile data from the collaborators, evaluate the quality of the submitted data before uploading them into the database. The action leader will follow up with contributors in case of misunderstandings, errors, or missing information in the submitted data. Additionally, a user test involving experts using the BADB will be organised to confirm the database's ease of navigation. If necessary, improvements to either the Data Collection Template or the user interface will be addressed.

A list of potencies of individual substances for different bioassay types (e.g. 'ERa receptor activation') will also be compiled in the final version of the database, in a dedicated sub-module. Furthermore, building upon the comprehensive study conducted by Kramer et al. in 2024 (https://www.nature.com/articles/s41597-023-02904-7) as part of the JPA 2023, information on the modes of action (MoA) will be available for more than 3,300 environmentally relevant chemicals. This valuable data will be integrated into the BADB in collaboration with WG-2. As a result, users will have the capability to evaluate the sensitivity of various assays to chemicals across different MoA categories. Additionally, we are planning to provide Effect-based Trigger Values (EBTs) for each bioassay with enough available data in a dedicated sub-module, leveraging the collected *in vitro* bioassay data, in analogy to the Quality target Module of the ECOTOX database.

As part of the next JPA (2025), our plan is to go beyond merely "compiling" information on bioassays responses, substances' potencies and Effect-based Trigger Values (EBTs). Once a critical mass of data becomes available, we intend to introduce a tool for deriving EBTs, in analogy to the existing "PNEC derivation module" in the ECOTOX database. Furthermore, in analogy with the CRED module, we aim to implement a mechanism for verifying the reliability of bioassay data, based on the provided metadata. This will be comparable to the established reliability scoring system thanks to alignment with the metadata from the SCIRAP tool.

WG-1 Prioritisation of CECs

Working Group N°1: Prioritisation of CECs (Activity coordinated by INERIS valeria.dulio@ineris.fr in collaboration with EI slobodnik@ei.sk, alygizakis@ei.sk and UBA peter.vonderohe@uba.de).

The prioritisation activities of WG-1 constitute an ongoing effort to integrate various NORMAN activities in alignment with the objectives of the EU Chemicals Strategy and the Zero Pollution Action Plan. The primary focus of WG-1 is two-fold:

- To ensure that all relevant information necessary for assessing chemical risks is consistently maintained and updated in a timely manner;
- To actively integrate and leverage this information to identify lists of chemicals requiring priority actions. Each priority list corresponds to a specific action.

In 2024 the focus of WG-1 will address the following topics:

Task 1: Support the prioritisation work of the Commission services at European level and provide comment on relevant consultation documents (PARC, EWS, where relevant) (ALL)
NORMAN participates as a stakeholder in the WG Chemicals of DG ENV and intends to further contribute to the activities related with the review of the list of WFD Priority Substances and the Watch List. In 2023 NORMAN WG-1 provided proposals for the 5th review of the Watch List. In 2024, NORMAN will be able to contribute to the PARC partnership on the following prioritisation-related topics:

- Collaboration in the development of a mechanism for priority setting in environmental and multi-source monitoring in the context of the MonitoringFrame project (PARC T4.2.b_Y2);
- Contribution to the review of existing data on EDCs and PFAS for the PARC pilot monitoring study;
- Early Warning System for Europe (EWS) NORMAN will contribute with NTS data from the DSFP, but also target monitoring data from EMPODAT and substance info (hazardous properties) from prediction models.

Task 2a: Collection and prediction of compound-specific information in support of prioritisation (UBA / EI / NKUA / DERAC / INERIS)

- Extraction and **compilation of experimental ecotoxicity data from** the REACH portal and UBA ETOX database;
- Retrieval of data on physico-chemical properties (e.g. Kow, Koc, BCF) as well as **hazardous properties (i.e. related to ED, CMR, PBT, PMT) from REACH registration dossiers and future CLP dossiers**. The collected data will feed the Substance Factsheets. For this purpose, it is planned to develop a dedicated Data Collection

Template (DCT). When experimental data is unavailable, prediction models will be developed and employed to address the gaps;
- Development of a **quantitative model for persistence,** based on a set of **8000 reported degradation half-lives for the OECD 302 tests**. The models will allow to **predict the DT50 in water for all compounds in SUSDAT** that are covered by the model domain;
- Assessment of the P, B, T, CMR and ED scores which were already assigned to 88,524 compounds in the SusDat list using the JANUS model. These scores are already integrated in the Substance Factsheets.

Task 2b: Group of Experts in Prediction models and Machine learning
- Organisation of focused meetings with a **Group of Experts in modeling and machine learning**. The objective is to achieve **consensus regarding the deployment of predictive models** within the context of NORMAN;
- **Development of a new General Application Domain (GAD)** to ensure that only reliable predictions are reported in the Substance Factsheets and used for the prioritisation of chemicals. The GAD should ensure that the prediction models are not overfitted, while structures that are clearly not covered by the model are detected with high confidence. **The modelling Expert Group should strive to achieve consensus regarding the implementation of the GAD.**

Task 3: Collection of existing PNECs and prediction of PNECs (UBA / EcotoxCentre / DERAC / EI)
- **Collection and compilation of regulatory quality targets for various matrices**, including re-use, soil and marine waters (continuation of the work of the previous years). The aim is to extend the scope of the current prioritisation scheme to new compartments, thereby allowing consideration of multiple lines of evidence from different compartments;
- **Extension of the scope of prediction models**: following the successful extension of prediction models to include 3 additional fish species, 2 crustaceans, and 1 insect species, it is proposed to further broaden the scope of prediction models. This extension aims to encompass both acute effects and chronic effects in fish, daphnia, and algae. These predictive models will be applicable to aquatic species with large experimental datasets. The final aim is to enable a more robust statistical approach for the derivation of freshwater P-PNECs and their subsequent conversion for application to other matrices, like sediments and biota, e.g. by using Koc and BCF (see task 2). Thereby, the use of chronic-based endpoints will allow the use of lower AF for the derivation of the P-PNEC. This approach is likely to be well-received by regulatory bodies that rely on the prioritisation outcomes from NORMAN;
- **Prediction of toxicity values for both,existing compounds and those that have recently been added to SusDat**, to be up to date with the list of Lowest PNECs. The upload of existing PNEC and the derivation of new PNECs will also include **MAC-EQS values.** This will allow the evaluation of peak exposure concentrations, such as those resulting from the German small water body monitoring project;
- Derivation of more robust **PNEC marine values** to support prioritisation of compounds in the **marine environment** (delayed from JPA 2023);
- **Coordination of the Group of Ecotoxicity Experts for derivation and approval of (i.e. vote) new or revised Lowest PNEC values** for substances of the SusDat list, with a specific focus on substances that were highly prioritised in EU projects using the NORMAN Prioritisation Framework. The aim is to **progressively replace predicted PNEC values for substances prioritised in Cat 3 and 5, by experimentally-based PNEC values**.

Task 4: Compilation of data / information regarding 'Use categories' and 'Chemical Functional Use' for all SusDat compounds (LCSB / UBA / INERIS / EI)
With the ever-growing number of NORMAN SusDat substances, it becomes inevitable to group them by 'Use category' and 'Chemical groups category'. Some effort has already been made by EI to derive 18 use categories using the labels of the SLE lists, which are already implemented in the SEARCH function of SusDat. The classification of the compounds is not trivial since each substance has often multiple uses and associated sub-classes. The different approaches applied for categorisation of the uses (e.g. by REACH, US EPA Dashboard, PubChem) are not fully harmonised. A strategy within WG-1 – in line with the on-going collaboration between NORMAN and PubChem – was already proposed in the previous JPA (see WG-1, JPA 2023). It is planned to take up this action plan and make it operational in 2024.

Task 5: Prioritisation framework: follow-up activities to apply the new workflow beyond the freshwater compartment and across compartments and for specific chemical groups (ALL)
The work in 2023 has focused on the finalisation of the paper, the development of the infrastructure (back-end) to implement the online prioritisation tool linking the compounds' data in SusDat, target monitoring data (EMPODAT), suspect screening data (EMPODAT-SUSPECT under construction) and PNEC values (ECOTOX database). This operation has represented an important computational challenge (big data) which has required the preparation of structured data and indexing methods, the testing and further optimisation of the IT technology to allow fast data processing. The focus of 2024 will be on:

a) **Development of the IT infrastructure (EI and ALL):** building upon the developed infrastructure it will be possible to establish the operational connection between target and suspect data by implementing the workflow used in the WW pilot study.
b) Application of the **prioritisation workflow** to the **list of candidate EDCs** provided by **PARC (collaboration WG-1 and PARC).**
c) Application of the **prioritisation scheme (target and SS) to different data collections** (JDS4, EMBLZS, LIFE APEX) representing as far as possible different environmental compartments: it will be possible to characterise the profile of the compounds across multiple environmental compartments and identify the priority compounds supported by multiple lines of evidence.
d) **Prioritisation of contaminants in soil (WG-1 and WG-7)**: the work on prioritisation of contaminants in soil will remain *in stand-by until a critical mass of soil datasets* is available in the NDS. The newly EU-funded project TerraChem is expected to feed new data points in the NDS in near future.
e) Identification of list of ranked SusDat chemicals relevant for **acquisition of their chemical standards or MS(MS) information** allowing for target screening **(Eawag, LCSB).** This is an ongoing effort which started with a first test in 2022 (UFZ). Thanks to the results of the application of the prioritisation workflow on multiple data collections it will be possible identify the overlaps in the priority groups. The final selection of a list of the "most wanted" spectra will consider the information available in NORMAN-SLE, PubChem and CompTox. Once purchased and measured, the data should become available in the NORMAN Database System (e.g. MassBank, NORMAN-SLE).

Task 6: Prioritisation of contaminants in reused matrices (WG-1 and WG-5):
In 2023, WG-5 revised the design of six EMPODAT DCTs to allow their application to reused matrices. New occurrence data based on literature review will be compiled in EMPODAT for reused practices, i.e. stormwater, reclaimed water and sewage sludge in 2024. Moreover, new quality targets for reused matrices in agricultural practices were collected and uploaded in the ECOTOX database and further quality targets in sewage sludge for agricultural fertilisation will be derived (Task 3 in WG-5). Thanks to this new input in 2024 it will be possible to start testing the NORMAN prioritisation workflow on the specificities of the reused matrices.

Task 7: Improvement of the features of the prioritisation tool (expert consultation and programming activities) (ALL) (task planned in previous JPAs) (EI, INERIS, UBA, UFZ, NKUA, OVAM, DERAC, LCSB, KWR)
Further additional options for improvement of the prioritisation tool have been discussed in the Database workshop in 2023 and within the Prioritisation WG-1. At the moment, the output of the prioritisation tool is a downloadable Excel file with the list of substances sorted by category and associated scores.
WG-1 proposes to explore the integration of unsupervised clustering as a new feature besides the conventional output (table) (e.g. Principal component analysis (PCA). Hierarchical clustering. Self-organising maps.
As regards the visualisation options, it will be possible to consider: Network analysis, Trends analysis, Heatmaps and Venn diagrams. All these tools will allow to draw more conclusions about the prioritisation results (beyond the action categories).

Task 8: New development of the prioritisation tool in collaboration with PARC (EI, INERIS, UBA, NKUA, UFZ, OVAM, LCSB)
The development of the **Prioritisation project in PARC** involved the start of a collaboration activity with WG-1. In the PARC project it was decided to create a system flexible for new prioritisation queries (regulatory and research needs). This would include the extension of the list of indicators and the possibility for the user to customise them, including the weight of each indicator for the scoring system. It was proposed that the NORMAN Database System could provide the infrastructure for the programming of the prioritisation tool proposed in PARC. If this option is confirmed, a new prioritisation tool will be developed and in the beginning it will co-exist with the current one. This task will be organised in two steps:

- Meetings (virtual, if possible 1 physical meeting) for consultation of the WG-1 experts and PARC: proposals / desk work to revise the features of the prioritisation tool;
- Programming work: expected to start in the second part of 2024 after agreement with the WG-1 experts, based on dedicated instructions derived by a smaller team of experts.

Task 9: State of the environment in Europe (task planned in previous JPAs) (EI, UBA, INERIS and ALL)
We would like to integrate the results of single substances risks at certain sites into a total effect, by mapping the concurrent occurrence of chemical contaminants in Europe, across compartments: e.g. “how many compounds exceed the lowest PNEC at each site?”, or “what is the total mixture risk at each site?” These might become new chemical indicators to measure progress in the quality of the environment e.g. as a result of remediation measures and inform policy decisions (cf. pesticides indicator of the EEA) about the trends. This would allow NORMAN to, e.g., support the Zero pollution monitoring report of the EEA.

WG-2 Bioassays

Working Group N°2: The value of bioassays and biomarkers in water quality monitoring programmes (Activity coordinated by Goethe University Frankfurt, Henner Hollert Hollert@bio.uni-frankfurt.de and Sarah Johann johann@bio.uni-frankfurt.de)

Task 1: Two-day workshop of WG-2
A WG2 workshop will be organised in summer of 2024. A broad range of topics will be discussed, including contributions of WG-2 to the bioactivity database, links between the bioassays and EDA activities in WG-3, innovative behavioural assays, eDNA-and (e)RNA based methods, including transcriptomics, adverse outcome pathways, as well as the future implementation of effect-based methods in European chemical regulations.

Task 2: Joint Publication
As a follow-up to the successful workshop on "Innovative Approaches for Environmental Monitoring of Chemical Pollution and Biodiversity – Linking Biodiversity Loss and Chemical Pollution" in December 2023, a joint manuscript is planned to be submitted as a NORMAN position paper. This manuscript should involve all workshop speakers as well as interested workshop participants. The main objective of this manuscript is twofold:

- Discussing the relationship between chemical pollution and biodiversity changes, while considering the implications of chemical pollution within the conceptual framework of planetary boundaries, EU strategies on biodiversity and chemicals, and sustainable chemical markets;
- Bringing together existing expertise and methods related to chemical pollution and biodiversity. This involves promoting cooperation, combining existing databases from both fields, and conducting joint studies.

Task 3: Research project on temporal trends for transcriptomics in effects assessment
Since 2005, suspended particulate matter (SPM) samples are systematically collected from major German rivers, including Rhine, Elbe and Danube for the German Environmental Specimen Bank (https://umweltprobenbank.de/en/, Zizka et al 2022, ESEU, https://doi.org/10.1186/s12302-022-00618-y and Fliedner et al. 2022, STOTEN, http://dx.doi.org/10.1016/j.scitotenv.2022.158430. The samples have been analysed for a range of inorganic and organic pollutants with target, cumulative and Non-Target Screening methods. In addition, DNA metabarcoding data from the SPM samples are available for fish and macrozoobenthos communities. Additionally, fish from the Environmental Specimen Bank have also been analyzed using transcriptomics.

The objective of this Joint Program of Activities (JPA) is to conduct a collaborative investigation on suspended particulate matter (SPM) from the environmental specimen bank using effect-based methods. Specifically:

- **Effect-Based Methods Evaluation**: selected effect-based methods from the NORMAN/SOLUTIONS biotest battery will be carried out on the extracted SPM samples;
- **Transcriptome and Behavioural Studies:** Simultaneously, extensive transcriptome and behavioural studies will be conducted on the early life stages of *Danio rerio* (zebrafish). This will allow us to compare the existing chemical exposure data of the SPM and the transcriptome data obtained from the exposed fish embryos, with the results of a comprehensive bioassays profiling.

In the planned project, extracts from the archived SPM samples will be used: 1) to expose the early life stages of *Danio rerio* and analyse gene expression using transcriptomics methods (eg Bluhm et al. 2014, DOI10.1371/journal.pone.0106523 and Reinwald et al. 2022, DOI10.1016/j.chemosphere.2021.132746). 2) to apply EBMs of the NORMAN/SOLUTIONS EBM battery (Brack et al.2019, ESEU, https://doi.org/10.1186/s12302-019-0192-2).

Task 4: Follow-up of activities started in previous JPAs
The work of WG-2 Bioassays in 2024 will also cover the following ongoing actions from previous JPAs:

- **Remobilisation of pollutants during extreme flood events** (Leader: Goethe University Frankfurt Hollert@bio.uni-frankfurt.de) ten sediment and suspended sediment samples, out of ca. 150 samples collected in the Eifel region further to the summer 2021 flood event, were selected for this study. The extracts were distributed to the 13 labs participating in this ring study for detailed and comprehensive toxicological and chemical profiling to evaluate the impact of such an extreme flood event in respect to the goals of the European Water Framework Directive. The evaluation and statistical analysis of the results by Goethe University have been completed. The WG-2 workshop in 2024 will provide participating labs the opportunity to meet and discuss the results, considering a joint publication as well as the elaboration of proposals for consideration in the implementation of the WFD. Finally, as agreed in the JPA, the project leader will feed the chemical and bioanalytical monitoring data in the NORMAN databases (EMPODAT and bioassays modules);
- **Ecosystem level effects of CECs on aquatic ecosystems (database / WG)** (Leader: Wageningen Environmental Research paul.vandenbrink@wur.nl in collaboration with IMDEA andreu.rico@imdea.org). A

paper presenting the outcomes of the NORMAN workshop*: Improving the use of (semi-)field data for the risk assessment of chemicals* (November of 2022) was under preparation in 2023 under the leadership of Paul van den Brink (WUR) and it is expected to be published in 2024;

- Development of ***in vivo* workflows to support explorative EDA studies** - solving bottlenecks using zebrafish (*Danio rerio*) and marine medaka (Leader: Goethe University Frankfurt Hollert@bio.uni-frankfurt.de and UFZ riccardo.massei@ufz.de). The main objective of this study (JPA 2020 – 2023) was to provide recommendations and guidelines for effective and fast *in vivo* testing in the context of EDA studies. The ultimate goal is to improve the application of *in vivo* bioassays in EDA studies for identification of CECs in freshwater. The activity has been successfully concluded. The Goethe University and UFZ teams could achieve the main goals described in the JPAs and a short communication on the main findings of this study was drafted and will be ready for submission early 2024.

Task 5: Support the work of the Commission (EBM – CIS WFD Activity) (Leader: Goethe University Frankfurt Hollert@bio.uni-frankfurt.de)
NORMAN WG-2 will continue to support the activities of the Commission as regards the implementation of Effect-Based Methods in the Water Framework Directive and other relevant directives.

WG-3 Effect-directed analysis

Working Group N°3: Effect-directed analysis for hazardous pollutant identification (Activity coordinated by UFZ Melis Muz, melis.muz@ufz.de and VU Frederic Béen, f.m.been@vu.nl)

Task 1: Contamination patterns, toxicity fingerprints and toxicity drivers of source-related effluents – Phase III – SOURCES project
In 2023 we will pursue and finalise the work started in the previous JPAs (2021-2023) for identification of source-related chemical and toxicological footprints (SOURCES project).

The research activities focused on *Identifying Source-Specific Contamination Patterns in Waste- and Surface Water using HRMS Data* have yielded promising preliminary results in 2023. Thanks to LC-HRMS technology, the chemical composition of each wastewater sample was successfully decoded. For each of the 93 samples across 8 source classes, a list of annotated features was obtained. By analysing variations in these features among different sources, it was possible to identify the distinctive features representative of specific source classes. Using this dataset, it was possible to develop and train a machine learning (ML) model for predictive analysis. Its purpose is to assign unknown samples to specific source classes. The results demonstrate that different sources emit unique chemical fingerprints into the environment. These findings highlight the critical importance of identifying and monitoring these patterns for enhanced environmental management.

Another aspect of the study focused on *Obtaining source-specific toxicity fingerprints*. Here, the alignment of the toxicity patterns with the source classes was more critical showing that the toxicity of source classes does not adhere to a consistent pattern; instead, it is driven by specific toxicants. Therefore, samples exhibiting pronounced effects for the tested endpoints were selected to identify the key toxicants driving these observed effects using HT-EDA. The first proof-of-case study was based on androgenicity as an endpoint. Further to HT-fractionation, toxicant prioritisation by application of *MLinvitroTox* models on non-target screening data has enabled a significant reduction in the number of relevant features to be processed for compound identification. Despite this progress, there may still be hundreds of potential candidate structures for a given assigned molecular formula. As part of the upcoming 2024 pilot project, it is planned to evaluate different computational tools for prioritising candidate structures based on specific endpoints.

Task 2: Integration of computational toxicity driver prioritisation tools to support non-target screening workflows in high-throughput effect-directed analysis
Further to the outcomes of the SOURCES project (Phase III) “Contamination patterns, toxicity fingerprints and toxicity drivers of source-related effluents”, in 2024 the main activities of the WG-3 will be dedicated to a new pilot project aimed at implementing the most promising computational tools to improve the efficiency of current compound identification workflows and adapt them to HT-EDA applications.

In the past few years, effect-directed analysis has made significant advancement in the direction of getting more high-throughput. These changes have been particularly marked by the automation and miniaturisation of fractionation, as well as the optimisation and downscaling of bioassays. High resolution mass spectrometry coupled to liquid chromatography and consequently non-target screening have been instrumental to improving the identification of novel risk driver compounds in aquatic environments. However, the current identification approaches have two main challenges two overcome: (i) prioritisation of features to be subjected to identification efforts among a list that comprises thousands of features, (ii) prioritisation of generated candidate structures of these selected features by in-silico fragmentation tools, which can reach hundred possible structures depending on the assigned molecular formula.

Recently, several computational tools have been developed supported by machine learning approaches in order to enhance toxicity prediction based on different available information such as ms2 spectra, candidate structure, ionisation behaviour...etc. We believe that many of the developed tools for toxicological endpoint prediction are perfectly suited to toxicity driver prioritisation and have not yet been explored in the context of EDA.

The activities for 2024 will be organised around three objectives:

Activity 1: Evaluate existing computational tools to prioritise candidate structures of toxicity drivers for application within non-target screening workflows adapted to EDA studies (supported by the info gathered for EDA review paper currently being written by the lead of WG3).

Activity 2: Computationally associate the structures in the NORMAN Suspect List to potential effects on the gene/pathway level for environmentally relevant endpoints such as estrogenicity, androgenicity, and neurotoxicity by using *deepFPlearn* (https://doi.org/10.1093/bib/bbac257).

Activity 3: Validate the efficiency of selected tools for prioritising potential toxicity driver features/structures using the data obtained in the SOURCES project as a starting basis. Mainly, we will assess whether the compounds prioritised with these tools can explain the observed toxicity of the selected SOURCES samples.

Activity 4: Establish optimal endpoint-specific toxicant identification protocols for HT-EDA that incorporate these tools and make them accessible to the rest of the community.

These activities will be carried out in close collaboration with JPA "Bringing together NTS and toxicity, *MLinvitro*, *MS2Tox* and other tools". This collaboration is driven by the fact that the some of the applied computational methods will be shared across the two studies.

Task 3: Organisation of a session at SETAC Europe 34th Annual meeting (5-9 May 2024) – "Novel Technologies for Toxicity driver Identification: Advances and Challenges in Effect-Directed Analysis and Beyond" (Melis Muz-Massei, Iker Alvarez-Mora and Frederic Been). NOTE: the proposed session has been merged with another session. The final title is: "*Complex Mixtures of Chemicals in the Environment and the Human and Eco-Exposome – Next Generation Monitoring (NGM), Toxicity Driver and Source Tracking to Meet Regulatory Needs*".

WG-4 Nano- and micro-scale particulate contaminants

Working Group N°4: Nano- and micro-scale particulate contaminants (Activity coordinated by Eawag – Ralf.Kaegi@eawag.ch and NIVA Bert.vanBavel@niva.no)

Task 1: ILS for the analysis of MP in environmental matrices using the upcoming ISO standard (in collaboration with ISO TG 147/SC2 /JWG1, and the PlasticTrace project)
Working group 4 has accomplished 2 JPAs (2022 and 2023) contributing towards NORMAN's general objective to enhance harmonisation approaches for measuring microplastic particles (MP). These efforts have been part of implementations in EU's Green Deal, the Plastic Strategy supported by EUs directives and risk assessment. The JPA in 2022 included an interlaboratory study (ILS) to detect MP in complex matrices which could benefit from a collaboration between QUASIMEME and the EU project EUROqCHARM. The results reported by the different laboratories showed a high variation, even for simple matrices. These variations were a combination between the uncertainties related to the sample preparation, and the uncertainties related to data processing pipelines. However, the experimental design of the ILS did not allow to distinguish between the two sources of uncertainties.

Within the last JPA (2023), WG 4 developed a sandwich filter to specifically address the uncertainty related to the data processing pipelines, and the robustness of the filters were tested by selected NORMAN members.

At the Annual WG4 meeting in June 2022 the need for further QA/QC studies was discussed. Harmonised methods are getting more mature and reference materials are under development to enhance the analysis of MPs.

Building on the experiences of the JPAs from 2022 and 2023, and considering the feedback from the NORMAN members, the activities of WG-4 in 2024 will be devoted to the organisation of a new ILS based on the upcoming ISO standard method for water samples. This method comes with a firm description of the sample preparation. For the study, NIVA and Chiron AS will manufacture soda tablets containing known amounts of different MP types (Polypropylene (PP), polyethylene (PE), polystyrene (PS), polyvinyl chloride (PVC), polyethylene terephthalate (PET) and polycarbonate (PC)). In addition, a limited number of 'sandwich filters' assembled at Eawag will be sent to expert laboratories taking part in the ILS. The ILS will be organised in collaboration with ISO TG 147/SC2 /JWG1, and the PlasticTrace project as part of the validation of the ISO method (ISO/NP 16094-2 *MP in water – Vibrational spectroscopy).

The work in 2024 will involve the following activities:

- **Organisation of the 4th round of the Microplastic ILS**

The fourth round of ILS for the analysis of MP in environmental matrices will be organised in a collaboration with the ISO/CEN organisation and the PlasticTrace project. The ILS will include triplicate analysis of soda tablets spiked with MP (PP, PE, PS, PVC, PET, and PC), in addition to blank tablets, produced by NIVA and Chiron. The participating laboratories will be required to use the ISO standard for water samples due to be distributed January 2024.

- **Comparison of different data processing pipelines**

'Sandwich' filters, spiked with different types of MP (PE and PS) of different sizes (50 – 100 µm) and of different colours will be sent to 10 expert laboratories, including NORMAN WG-4 members, participating in the ILS. The laboratories will be provided with the filters and will be asked to analyse the particles on a given fraction on the filters, in addition to processing the data. The laboratories will be asked to report the key instrumental and software parameters, in addition to the number, size, and type of identified MPs.

- **Workshop for evaluation of the results of the ILS**

A workshop will be held to evaluate the results of the ILS, in connection with WG-4 annual meeting. In addition to this, a special webinar will be organised to reach a larger group of stakeholders (autumn 2024).

Task 2: (Micro)plastics – leaching of additives and non-intentionally added substances (NIAS) (Leader: TNO andrea.brunner@tno.nl . NKUA, nalygizakis@chem.uoa.gr). This task will be organised in collaboration with the NTS-CWG (see Section (Micro)plastics – leaching of additives and non-intentionally added substances).

Task 3: Follow-up activities previous JPAs

- **Reference material and standards for micro- and nano-plastic research** (Leader: NIVA Bert.vanBavel@niva.no and Eawag – Ralf.Kaegi@eawag.ch)

This activity addressed the development of micro- and nano-polymer reference materials for the ILS organised in collaboration with QUASIMEME. The material has been used for round 2 (2021) and 3 (2022) of the ILS. Small MPs (< 10 µm) and nano particles of the most commonly used polymers were produced by fragmentation at NIVA and further separated into (nano-size) fractions, but they could not be produced in large quantities. A summary report will be submitted to NORMAN on the results of the production of the different reference MPs in 2024.

Based on the results of this task, PP and PET were selected for further evaluation of the production of a reference material at NIVA. Microplastics of the most commonly used polymers, i.e. polyethylene (PE) polypropylene (PP), polyamide or nylon (PA), polyethylene terephthalate (PET), PS (polystyrene) and PVC (polyvinylchloride) will once again be produced in 2024. This production aims to support the ILS scheduled for the same year.

WG-5 Water reuse and policy support

Working Group N°5: Water reuse and policy support (Activity coordinated by DERAC, France genevieve.deviller@derac.eu in collaboration with LTU, Sweden lian.lundy@ltu.se).

A growing interest for data on biological and chemical contaminants of emerging concern (CECs) linked to reuse practices (i.e., the use of wastewater and associated sludge for different purposes e.g. agriculture, aquifer recharge, support public health decision-making, urban and recreational activities, construction, land restoration) has emerged with the Circular Economy Action Plan, the recent adoption of the new EU regulation on water reuse for agricultural irrigation and revision of the EU Directives related to urban wastewater treatment and the use of sewage sludge in agriculture.

In line with the proposed activities built on the WG-5 mandate, three projects, all related to databases, are planned to continue in 2024.

Task 1: The Antibiotic Resistance Bacteria and Genes Database

NORMAN ARB&ARG was first launched in 2021 as an open platform for the exchange of ARB&ARG occurrence data and analytical methods following the FAIR (Findable, Accessible, Interoperable, Reusable) principles. The database has been enriched with 2622 data points from 11 countries (795 soil, 595 surface water, 705 groundwater, 484 wastewater, 43 sewage sludge). An overview of the database functionalities, data extraction, and the contribution of data to the database has been presented in a manuscript currently under peer-review evaluation. The ambition to collect enough data to establish baseline ARB&ARG concentration levels in soil, wastewater, sludge, groundwater, and surface water still remains a primary goal. The goals for 2024 are as follows: 1) Intensify efforts to collect, harmonise, and upload ARB&ARG data from key scientific publications, 2) Improve the visualisation capabilities of the database, 3) Attempt to initialise a monitoring campaign for ARB&ARGs and A&TPs to enrich the database with new data, and 4) Investigate the incorporation of NGS data into the database.

Overall, there is great potential for scientific breakthroughs with the ARB&ARG database. However, it is important to recognise that there are on-going parallel initiatives outside NORMAN aiming at building Databases on ARB&ARG. NORMAN WG-5 will therefore ensure that there is a critical mass of data suppliers for the NORMAN ARB&ARG database. WG-5 will strive to align efforts with other organisations such as the Technical University of Dresden, University of Thessaly, and a few others to strengthen NORMAN's position regarding these contaminants.

Task 2: the SARS-CoV-2 in sewage (SC2S) Database
Whilst several countries launched national SARS-CoV-2 in wastewater databases to share information on viral concentrations during the pandemic, the NORMAN SARS-CoV-2 database is the only online, open access database sharing data from multiple countries and hence remains a useful research resource currently hosting over 1000 data sets from 11 countries.

Results obtained in 2023.
A joint meeting was held with the SCORE network to brainstorm ideas for the future of the database. The decision was made to undertake a survey among NORMAN and SCORE members with a view to understanding current wastewater-based epidemiology activities linked to infectious diseases. Survey results will be used to extend the remit of the SARS-C0V-2 database to additionally host data on other infectious diseases.

Activities planned for 2024 (in-kind contribution).
- Undertake a survey to explore the possibility to expanding the database to include e.g. influenza and RSV and rebrand the database at the 'infectious diseases database';
- Invite contributions from NORMAN- and external organisations to upload historic SARS-CoV-2 WW data into database (the publication of a paper could be proposed as an attractive opportunity).

Task 3: Databases for CEC risk characterisation in reused environmental matrices
The risks linked to chemicals in reused matrices like water and sewage sludge are mostly unknown and occurrence data as well as quality targets (or threshold values) are needed to characterise and prioritise those risks. Therefore, the WG-5 have identified as a new priority the collection and the dissemination of such data to support research projects, policy makers and environmental managers. This initiative is supported by the Water Europe Zero Pollution Working Group.

The opportunity to upgrade the NORMAN existing databases, EMPODAT for occurrence data and Ecotoxicology for quality targets (hazards data), was identified in 2021 as the most relevant approach to collecting data related to chemical contaminants in reused matrices and to characterise their risk according to the WG1 prioritisation framework. In 2023, the following tasks has been performed to reach this objective:
- Upload of six new EMPODAT DCTs (WWTP, surface water, groundwater, sediment, soil, biota) on the NORMAN website with new matrices (e.g. reclaimed water, stormwater, stormwater pond sediment, dredged sediment, excavated soil) and reuse categories (e.g. agriculture, aquifer recharge, recreational and urban activities…);
- Compilation of Canadian regulatory quality targets for water reused in agriculture in DCT for Ecotoxicology database and upload in the WG5 private area on the NORMAN website;
- Collection of quality targets in soil and the conversion of quality targets for sewage sludge reused in soil fertilisation;
- Risk characterisation of pesticides and metals in different water types reused in agriculture;
- Risk characterisation of CECs in stormwater, WWTP effluents and reclaimed water reused in agriculture and surface water recharge (on-going).

The activities planned for 2024 are the following:
- Collection and publication of new occurrence data (at least 1000) based on literature reviews, focusing on stormwater, reclaimed water and sewage sludge which are currently missing in EMPODAT;
- Collection and publication of new quality targets on soil and conversion in quality targets on sewage sludge for agricultural fertilisation in the Ecotoxicology database;
- Perform the risk characterisation and prioritisation of CECs in sewage sludge for agricultural fertilisation;
- Publish the risk characterisation and prioritisation of CECs in reused waters including stormwater and reclaimed water in a peer-review journal.

WG-6 CECs in the indoor environment

Working Group N°6: CECs in the indoor environment (Activity coordinated by RECETOX lisa.melymuk@recetox.muni.cz in collaboration with NILU Pernilla.Bohlin.Nizzetto@nilu.no. VU pim.leonards@vu.nl and University of Antwerp adrian.covaci@uantwerpen.be).

Task 1: Combining Wastewater-Based Epidemiology and indoor dust analysis for comprehensive evaluation of chemical exposure risks in indoor environment (Leader: University of Bath, Barbara Kasprzyk-Hordern bkh20@bath.ac.uk, UFZ, saskia.finckh@ufz.de, Sara Castiglioni, Istituto Mario Negri, sara.castiglioni@marionegri.it, RECETOX, Lisa Emily Melymuk, lisa.melymuk@recetox.muni.cz)
Wastewater represents a fingerprint of a city's metabolism. It is a complex mixture of substances of biological and chemical origin including indoor environment community stressors such as hazardous chemicals and their human transformation products. The quantitative measurement of these substances continuously pooled by the water system can provide evidence of community-wide exposure to these chemicals. While wastewater is a source for environmental pollution in NORMAN, the extension of wastewater screening as a proxy for domestic exposure (e.g. from indoor environment) will provide a valuable benefit for the identification and prioritisation of hazardous chemicals, which is a major focus of NORMAN. This approach also helps to better link the efforts of WG-6 on indoor environments to the water related activities in NORMAN and provides relevant data for NORMAN databases. Water-based chemical mining (also known as WBE – Wastewater Based Epidemiology) utilising metabolic biomarkers of exposure and effects that are produced collectively by studied populations and ultimately end up in urban water, provides a timely complimentary tool to traditional biomonitoring approaches. Similarly, chemicals emitted indoors are present in indoor air and dust, which is yet another, important matrix enabling chemical exposure studies.

This proposal aims to combine the investigation of indoor environments (DUST) and human community exposure via wastewater analysis (WBE) to provide a new, holistic framework for comprehensive understanding of human exposure risks to hazardous chemical mixtures in indoor environments. This will be done via an integration of three key ongoing activities in Europe:

- WBE pan-European monitoring program planned in 2024 in PARC (4.3_E01 - Mining chemical information in wastewater for human community and environmental exposure assessment);
- SCORE network activities focused on annual WBE monitoring campaigns;
- NORMAN WG-6 on Indoor environments and ambient air.

The tasks and objectives planned for 2024 include:

- Mapping cities/countries and timescales for samples already collected/analysed across Europe Mapping cities/countries with existing WBE and DUST databases across Europe (mainly within Norman, SCORE and PARC projects);
- Identification of common targets and verification of associations between chemicals in dust vs wastewater;
- Writing a perspective paper on opportunities in human exposure studies, also in the "One Health" context via combined monitoring encompassing both WBE and DUST frameworks. We aim to come up with a solid framework for WBE-DUST within one year;
- Organisation of the Workshop (end 2024).

Task 2: Follow-up tasks started in the previous JPAs, as listed below.

- **CT on Passive air sampling and wide-scope suspect/non-target screening for organic substances in air (in collaboration with PS-CWG)**
  A preparatory workshop and deployment of the passive PDMS foam sampler adsorbents are planned for the first half of 2024. Exposed samplers will be distributed to the participants by the fall of 2024. Extraction and analyses to be done by labs with a deadline by early 2025;
- **2nd CT on non-target and suspect screening methods for organic substances in European indoor dust**: Data analysis of GC-MS and LC-MS data has been completed. A scientific paper is planned for autumn 2024 (Action leader: peter.haglund@chem.umu.se Umeå University);
- **Geographical distribution of organic substances in European indoor dust**: Extracts of house dust were distributed among laboratories that have volunteered for analysis. All of the analyses have been completed and the results have been compiled. A scientific paper is planned for autumn 2024 Most likely, this will be a collaborative paper that combines findings from both the collaborative trial and the geographic distribution study. (Action leader: peter.haglund@chem.umu.se Umeå University);
- **Intercomparison study of dust sampling methods**: In line with the initial plan, this study will analyse chemicals from the following groups: chlorinated paraffins, POPs, plasticizers, and OPFRs. In 2021, two datasets were finalised – chlorinated paraffins and POPs. However, the samples assigned for analysis of plasticizers and PFRs

by the University of Antwerp are still pending dispatch from VU. A joint publication is envisaged (2024) (Action leader: pim.leonards@vu.nl VU).

WG-8 Marine environment

Working Group N°8: Marine environment (Leader: DCU fiona.regan@dcu.ie in collaboration with Marine Institute Brendan.McHugh@Marine.ie)
WG-8 on Marine Environment plays a pivotal role within the NORMAN network. Since 2020/2021, this group has gathered a multi-disciplinary community of experts from academia and environmental agencies, all active in the field of contaminants of emerging concern in the marine environment.

In November 2022, the WG-8 kick-started its activities under the joint leadership of DCU and the Marine Institute. Prior to this, collaborative initiatives had already been launched, as part of the previous Joint Programming Activities (JPAs), in connection with co-funded projects e.g., EU-funded LIFE APEX and EU/UNDP-funded EMBLAS-Plus and EU4EMBLAS. These research initiatives have been instrumental in demonstrating the added value of the approaches developed by the NORMAN network in support of the implementation of the Marine Strategy Framework Directive (MSFD), including non-target screening, passive sampling, substance prioritisation, marine ecotoxicity threshold values and monitoring of microplastics.

In 2023, the efforts of WG-8 were successful in formally establishing the working group, which today counts more than 30 registered experts and organisations. To promote the long-term cohesion of the group, WG-8 participants have committed to developing a 5-year roadmap, defining the strategy of the WG regarding the priority topics to be addressed in the coming years and the links with the other NORMAN WGs and communities outside the network. In the first year, the following practical tasks were identified: 1) Prioritisation of sea-specific contaminants for the four European Sea Regions; 2) Systematic sharing of published and proposed marine biota, water and sediment ecotoxicity threshold values for inclusion in the NORMAN Ecotoxicology Database; 3) Scoping of new activities; 4) Collaboration with OSPAR and HELCOM on monitoring, trends and effects of substances in the marine environment. These steps will pave the way for the following years, during which the roadmap will be refined and expanded.

Thanks to the meetings organised in February, April and November 2023 the participants were able to discuss the key challenges for prioritisation of sea-specific contaminants, based on the experience from the four European Sea Regions, HELCOM and OSPAR, the final goal being the generation of a robust prioritisation framework for CEC in the marine environment. The exploratory discussions recognise that methodologies can be different, but we can all learn from the processes. A discussion was had regarding risk assessment and the steps required in establishing a framework for prioritisation. A call for publications has been sent to members, requesting the submission of relevant publications on CECs in the marine environment and legacy pollutants as well as for relevant data sets.

The activities planned for 2024 will be organised around the following tasks.

Task 1: WG Coordination
- Meetings: It is planned to hold monthly meetings between February and November. All Norman members will be informed and will have the opportunity to participate. The aim is to agree on the workplan and gather smaller groups to address each of the tasks;
- Newsletter and website updates: We will request information from members monthly to generate bi-monthly newsletters and content for the website to have a go-to-place for members. We will provide (as in 2023) an easy template for gathering publications and data;
- WG 8 roadmap: Development of 5-years roadmap covering all relevant topics identified by the WG and links with other WGs, in particular, key aspects related to prioritisation/identification of sea-specific pollutants, mixtures risk assessment, microplastics, status indicators to monitor the changes of the marine environment, optimisation of monitoring strategies (use of non-target screening, bioassays, passive sampling);
- Sub-groups for working on tasks 2 and 3 will be established and will meet as needed;
- The WG will consider the possibility of organising a marine environment presentation or mini seminar at the next GA meeting.

Task 2: Prioritisation of sea-specific contaminants for European Sea Regions
The proposal is for prioritisation of substances identified/determined in the North-East Atlantic and Baltic Sea under a series of tiers (using the NORMAN Prioritisation Framework as a starting basis):

- Tier 1: OSPAR CONNECT, OSPAR CONNECT2 and HELCOM PreEMPT projects;
- Tier 2: LIFE APEX, UBA-HELCOM, OSPAR CONNECT, OSPAR CONNECT2 and HELCOM PreEMPT projects;
- Tier 3: Reporting of ICES monitoring data to the NORMAN database;
- Tier 4: LIFE APEX, UBA-HELCOM, OSPAR CONNECT, OSPAR CONNECT2 and HELCOM PreEMPT projects.

any other data. This is contingent on completing Tiers 1 - 3 and required monitoring data from ICES incorporated into the database.

Moreover, in collaboration with WG-1, all marine samples (with a specific focus on biota and sediment matrices) will be retrospectively re-run with a list of >95,000 suspects in DSFP for presence of these substances in GC-HRMS and LC-HRMS chromatograms. The data will be uploaded in the EMPODAT SUSPECT database. The new NORMAN Prioritisation tool using target and wide-scope target data / suspect screening will be implemented for determination of priority substances for different action categories. We need to consider a number of technical aspects in terms of metals inclusion in this or future prioritisation schemes.

The WG will also investigate adjustments of the prioritisation scheme taking into account the specificities of the marine environment. Besides the classical Frequency of Appearance (FoA) and Frequency of Exceedance of PNEC (FoE), alternative indicators taking into account persistence and bioaccumulation properties of the substances, will be explored for integration in the prioritisation framework specific to the marine environment. The definition of marine mammal ecotoxicology values is a key issue for marine environment and such values should be obtained systematically. WG8 will aim to work closely with HELCOM and OSPAR initiatives in the field of ecotoxicology. The integration of the KEMI Exposure index will also be considered. The use of passive sampling data could also bring an additional line of evidence for prioritisation studies.

Connected with this activity there will be also work done for:

- Inclusion of the newly identified substances into the prioritisation workflow and uploading of the list in the NDS SLE;
- Optional: purchase of chemical standards of the top 50 GC-amenable substances. analysis by GC-HRMS, upload of mass spectra into MassBank Europe.

Task 3: Data gathering
An effort will be made to improve the population of the databases with the data relevant to the marine environment, with a specific focus on data from AMAP study on emerging substances in Arctic environment, data from the ICES database into LIFE APEX and NORMAN Database System.

Task 4 Ocean Decade event (timeframe in line with Joint Danube Survey 5)
WG-8 proposes to establish a Norman WG8 sub-committee to plan an Ocean Decade event on chemicals. This should also include members of ERICs and other relevant groups. The suggested timeframe should be in line with the 5th Joint Danube survey.

Task 5: Microplastics
We will meet quarterly with the microplastics WG to investigate how the harmonisation of reporting can be done and how microplastics screening could be achieved.

Task 6: Explore a MC DTN application for November 2024
It is proposed to prepare an application for a MC Doctoral Training Network building on the HORIZON 2020 project proposal which was not accepted in 2023.

WG-8 Monitoring, trends and effects of substances in the marine environment of the North-East Atlantic (OSPAR Commission)

Monitoring, trends and effects of substances in the marine environment of the North-East Atlantic (Leader: OSPAR Commission. contact person Brendan.McHugh@Marine.ie, Marine Institute)

Based upon the initial discussions at MIME 2019 and the list of identified areas for collaboration between OSPAR and the NORMAN Association, HASEC agreed to collaborate with NORMAN inter-sessionally, to prevent pollution by hazardous substances, by eliminating their emissions, discharges and losses, to achieve levels that do not give rise to adverse effects on human health or the marine environment, with the ultimate aim of achieving and maintaining concentrations in the marine environment at near background values for naturally occurring hazardous substances and close to zero for human made hazardous substances.

With this task, OSPAR's Working Group on Monitoring and on Trends and Effects of Substances in the Marine Environment (MIME) will ensure an effective collaboration with NORMAN linked with the following actions:

- CONNECT project and other project initiatives;
- Ecotoxicology;
- Passive sampling;
- List of chemicals for priority action and its annex;

- Chemicals in top predators and in polar regions.

The institutional collaboration in between OSPAR and NORMAN supports the implementation of the Northeast Atlantic Environmental Strategy 2030, specifically:

- S2.O1: By 2022 OSPAR will introduce a revised approach to managing the OSPAR Lists of Chemicals for Priority Action and Substances of Possible Concern (LCPA and LSPC). By 2022 and regularly thereafter, OSPAR will identify contaminants of emerging concern for the marine environment and prioritise them for action, including promoting and where necessary supplementing measures under relevant EU legislation and international organisations;
- S2.O2: OSPAR will develop and identify marine-relevant assessment criteria for hazardous substances, for use in the Quality Status Report 2023 and subsequently further develop these, including for emerging contaminants, working closely with relevant experts, particularly in the Working Group Chemicals under the Water Framework Directive Common Implementation Strategy.

CWG-NTS Non-target Screening Cross-Working Group Activity

CWG-NTS: Cross-Working Group Activity on Non-target Screening (Activity coordinated by Eawag juliane.hollender@eawag.ch in collaboration with EI slobodnik@ei.sk, University of Athens Nikolaos Thomaidis, ntho@chem.uoa.gr, LCSB - Luxembourg emma.schymanski@uni.lu).

In 2023, the NTS-CWG achieved significant milestones. The NORMAN guidance on Suspect and Non-target screening in environmental monitoring was published thanks to a collaborative effort involving numerous NORMAN experts under the leadership of Eawag and LCSB (*Hollender et al., 2023* DOI: 10.1186/s12302-023-00779-4). This guidance document serves as a crucial resource for decision-makers and stakeholders including PARC and its activities related to innovative methods. It represents a significant step forward towards the integration of suspect and non-target screening in chemical management and regulation. Additionally, NTS-CWG successfully disseminated the results of the Collaborative trial on suspect and non-target screening of organic micropollutants in biota, using LC and GC HRMS techniques under the leadership of SLU (*Wiebke et al., 2023* DOI: 10.1016/j.envint.2023.108288). This achievement contributes to advancing our understanding of the current performance of NTS techniques in complex environmental matrices such as biota.
Furthermore, under the leadership of QAEHS, we accomplished the task of compiling PFAS suspect HRMS lists and assessing PFAS-containing products. The outcomes of a comprehensive literature search and a survey involving 25 participants from 14 countries have been published in a short communication (*Dewapriya et al., 2023* DOI: 10.1016/j.hazl.2023.100086).

The following actions will be carried out as part of the CWG-NTS Activity in 2024:

- NORMAN Suspect Lists Exchange (LCSB) (see “NORMAN-SLE” above);
- NORMAN SusDat database: Database development and maintenance (EI, NKUA) (see “NDS”);
- Digital Sample Freezing Platform upgrading (EI) (see “NORMAN DSFP”);
- Finalisation and testing of EMPODAT – SUSPECT database - a new NDS module to host suspect screening results (EI) (see “WG-1 – Task 5”);
- MassBank Europe - Continuous development and upgrade (LCSB, Eawag and IPB Halle) (see “MassBank”);
- Machine learning-supported algorithms for assessment of the spectral quality and diagnostic information of MS2 data acquired with LC-ESI-HRMS (VU, UBA) (see “Assessing the spectral quality and diagnostic information of MS2 data acquired with LC-ESI-HRMS”);
- Integration of computational toxicity driver prioritisation tools to support NTS workflows in HT-EDA (EAWAG, EI) (see “Bringing together NTS and toxicity – Cooperation between *DSFP* and *MLinvitroTox*, *MS2Tox* and other tools”);
- (Micro)plastics – leaching of additives and non-intentionally added substances (NIAS) (TNO. NKUA) (see “(Micro)plastics – leaching of additives and non-intentionally added substances”).

Follow-up of activities started in previous JPAs 2019-2023:

- **CT on Passive air sampling and wide-scope suspect/non-target screening for organic substances in air (in collaboration with PS-CWG)**
  A preparatory workshop and deployment of the passive PDMS foam sampler adsorbents are planned for the first half of 2024. Exposed samplers will be distributed to the participants by the fall of 2024. Extraction and analyses to be done by labs with a deadline by early 2025;
- Collaborative Trial for the intercomparison of Ion mobility separation data (SLU). Progress of the tasks, as of December 2023: reference compounds have been selected. the extracts have been distributed to the participating laboratories. the data collection template has been developed and reporting of the results is ongoing (see

"Collaborative Trial for the intercomparison of Ion mobility separation data. Development of open-access CCS databases for IMS" – follow-up from JPA 2023);
- Expanding and validating the chemical space of non-target screening workflows (NKUA). Progress of the tasks, as of December 2023: the models have been developed. the team is working at drafting of a paper presenting the features of the models. There is a delay in the organisation of the trial (see "Expanding and validating the chemical space of non-target screening workflows" – follow-up from JPA 2023);
- **Intercomparison study on PS and suspect and NTS for PFASs** (QAEHS / RECETOX / VU). Phase I is well advanced and Phase II will be launched in 2024 (see "PFAS - Intercomparison study on passive sampling and NTS – Phase II");
- **Collaborative trial on (semi-)quantitative non-target analysis with LC/ESI/HRMS** (SU and NKUA) (see "CT NTS semi-quantification" JPA 2020). In October 2021, 9 water samples were sent to 46 laboratories around the world. Progress of the work (as of December 2023): the leaders of the activity completed the quality check and reprocessing of the contributed data in order to obtain unbiased results. The results of the activity and a peer-reviewed publication are planned for 2024;
- **Development of the NORMAN GC-HRMS workflows** (NKUA, NILU and EI) (see "NORMAN GC-HRMS workflows" JPA 2021): Prioritisation of GC-amenable compounds was finalised in 2022: a reproducible prioritisation of GC compounds based on real occurrence data was achieved and the prioritised substances were supplemented with additional substances based on the literature. Acquisition of reference standards is ongoing. Development and testing of MS-DIAL-based workflow to produce GC-HR-MS spectra is ongoing. Expected presentation at GA 2024. The GC functionality for DSFP was programmed and successfully tested. Aim is to have all spectra uploaded to MassBank by the end of 2024;
- **2nd CT on non-target and suspect screening methods for organic substances in European indoor dust**: Data analysis of GC-MS and LC-MS data has been completed. A scientific paper is planned for autumn 2024 (Action leader: peter.haglund@chem.umu.se Umeå University);
- **Geographical distribution of organic substances in European indoor dust**: Extracts of house dust were distributed among laboratories that have volunteered for analysis. All of the analyses have been completed and the results have been compiled. A scientific paper is planned for autumn 2024 Most likely, this will be a collaborative paper that combines findings from both the collaborative trial and the geographic distribution study. (Action leader: peter.haglund@chem.umu.se Umeå University).

CWG-PS Passive Sampling Cross-Working Group Activity

CWG-PS - Passive Sampling Cross-Working Group Activity (Activity coordinated by NIVA Ian.Allan@niva.no and INRAE cecile.miege@inrae.fr)

The following actions will be carried out as part of the CWG-PS Activity in 2024:

Task 1: One-stop shop for passive sampling (DCU fiona.regan@dcu.ie. Marine Institute Brendan.McHugh@Marine.ie) (updated from previous proposal in JPA 2022)

This activity seeks to develop a "one-stop shop" approach to collate relevant passive sampling study information into a central repository. The idea is that the work should not overly focus on the collation of analytical data itself but more so on key validation / modelling information underpinning these studies (e.g. scope of analysis, robustness, the influence of biofouling, Kpw etc) for a wide range of passive sampling techniques.

The one-stop-shop is expected to fulfil the following demands: (i) Provide a template for collection of passive sampling key performance criteria, (ii) Assemble relevant information, linked to papers, to potentially promote PS – identifying for example suitable case studies, (iii) Create a repository for this information compatible with the requirements of existing data management systems so that sharing is somewhat seamless, (iv) Critically assess key performance criteria in relation to passive sampling, (v) Promote the reporting of PS information, (vi) Create synergies with RSC and ICES working group activities, and (vii) Identify research gaps and needs.

A call for publications was released to PS CWG members in August 2023, with the opportunity for members to upload their relevant papers to a shared driver, allowing the working group to have access to the publications made available by fellow colleagues. At the end of 2023 63 publications had been collected and added to the shared folder.

With this in mind, goals and activities planned for 2024 include:

- Investigating text mining of the collection of papers assembled in 2023 (e.g. with tools such as used in PARC T8.2) and licensing issues;
- Deciding the longer-term goals of this compilation of PS papers;
- A Collaborative effort focusing on upgrading the PS database of the NDS addressing in particular: 1) populating the PS database (some datasets have already been identified - e.g. from Irish research studies – and they will be uploaded as a proof of concept; 2) developing links between the PS database and the other modules (passive sampling data could be used as an additional line of evidence for prioritisation of substances / sites); 3)

investigating the possibility of integrating uptake rates to derive concentration levels in water from concentration in PS.

Task 2: Intercomparison study on passive sampling and NTS for PFASs (Leader: QAEHS k.sarit@uq.edu.au in collaboration with RECETOX branislav.vrana@recetox.muni.cz, NIVA Ian.Allan@niva.no and University of Amsterdam s.samanipour@uva.nl) (see "PFAS - Intercomparison study on passive sampling and NTS – Phase II")

Task 3: Standardisation of passive sampling techniques for implementation in monitoring programmes (Leader: University of Limoges, sophie.lissalde@unilim.fr)
A satellite event will be organised on 15th May as part of the 14th IPSW 2024 (12-15th May, Limoges, France). The 13th IPSW in 2022 (Utrecht) highlighted the need for improved communication between scientists and policy-makers. Policy-makers and environmental agencies involved in the Water Framework Directive monitoring, discussed their expectations. The need for harmonisation and normalisation of passive sampling methods has been underlined. Following this, the 15th IPSW offers a dedicated session to continue this discussion taking advantage of the presence of many researchers involved in passive sampling. Selected researchers and policy/decision-makers will be invited to discuss harmonisation of passive sampling procedures and some key issues raised at the previous IPSW.

NORMAN PS-CWG seems an ideal actor to lead this exchange between decision-makers and the scientific community. The PS-CWG has a good overview of small or large-scale passive sampling projects that have been conducted in recent years across Europe and has been promoting the use of passive sampling for water quality monitoring. The group has been involved in the last 5-10 years in a number of actions related to this subject, including stakeholder-researcher workshops in Brno (2013), in Lyon (2015) or Prague (2016). The PS-CWG led an online meeting aiming to discuss the inclusion of passive sampling within biota monitoring strategies. In 2022, they also organised a one-day workshop on challenges to use PS for regulatory WFD monitoring. The final is to make a step forward towards the implementation of passive sampling in the water quality monitoring regulatory framework.

Follow-up of activities started in JPA 2020/2021

- Position paper on "Passive sampling in support of chemical monitoring in biota under the WFD (ongoing). An advanced draft has been developed by the core group of authors and it is expected to be submitted during the course of 2024.

CWG-NTS Bringing together NTS and toxicity – Cooperation between DSFP and MLinvitroTox, MS2Tox and other tools

Bringing together NTS and toxicity – Cooperation between DSFP and MLinvitroTox, MS2Tox and other tools (EI, Nikiforos Alygizakis alygizakis@ei.sk in collaboration with Eawag, Kasia.Arturi@eawag.ch, UFZ, SU, UBA, Peter.VonderOhe@uba.de) and other interested partners

Analytical laboratories routinely conduct daily measurements employing high-resolution mass spectrometry (HRMS). Despite advancements in target and suspect screening workflows, a significant proportion of signals detected in samples remain unidentified, posing a challenge to comprehensive chemical analysis. This challenge prompted NORMAN laboratories to organise and share the HRMS data with the scientific community, a task facilitated by the Digital Sample Freezing Platform (DSFP). DSFP processes the data through an optimised and standardised workflow generating component lists that retain all useful analytical information from the mzML files, including the HRMS/MS spectra of isolated precursor ions. Within these spectra lies valuable information about unidentified chemicals. Recent demonstrations have highlighted the use of fragmentation information in conjunction with machine learning models to predict toxic effects. Employing this approach seeks to enhance the understanding of chemical effects, a task that remains challenging even for well-known endpoints when considering only target compounds. This strategy aids in the prioritisation of unknown substances and also holds the potential to increase the percentage of explained effects, contributing to a more comprehensive understanding of chemical impacts.

The activities planned for 2024 and the expected outcomes are described below.

The proposed activity serves as an early-warning system for chemicals and their potential impact. Leveraging HRMS data obtained from the Joint Danube Survey 4 (JDS4), known for its comprehensive characterisation, we aim to employ a two-pronged approach. First, we will aggregate existing target and suspect screening chemical occurrence data and evaluate their contribution to measured effects using MLinvitroTox, MS2Tox and other tools.

Subsequently, we will analyse spectra of *unknown compounds* in JDS4 data stored in DSFP. This will allow us to predict the contributions of the *unknown fraction* to the overall effects and discern the drivers of specific endpoints within complex mixtures. Our strategy is expected to increase the percentage of explained effects and highlight the contributions from unknown components. This activity, functioning as an early-warning system, holds the potential to identify specific signals indicative of chemical hazards. If a limited number of signals prove relevant, we can proceed with a full identification workflow. Our overarching goal is to utilise advanced hazard tools and tap into the wealth of

component lists stored in DSFP. This comprehensive approach, if applied at large scale, ensures not only effective monitoring but also the potential for early intervention and risk mitigation in the realm of chemical impact assessment.

These activities will be carried out in close collaboration with WG-3 "*Integration of computational toxicity driver prioritisation tools to support non-target screening workflows in high-throughput effect-directed analysis*". This close collaboration is justified by the fact that some of the applied computational tools will be shared across the two studies.

CWG-NTS (Micro)plastics – leaching of additives and non-intentionally added substances (NIAS)

(Micro)plastics – leaching of additives and non-intentionally added substances (NIAS) (Leader: TNO, TNO andrea.brunner@tno.nl . NKUA, nalygizakis@chem.uoa.gr).

Plastic pollution poses a significant threat to our ecosystems, with microplastics and leaching of chemicals from micro- and macro-litter contributing to the complexity of environmental contamination. Traditional monitoring methods often overlook emerging contaminants, necessitating a comprehensive untargeted approach to identify and understand the impact of plastic additives and other plastic associated chemicals. High-resolution mass spectrometry (HRMS) has emerged as a powerful tool for detailed chemical analysis. This proposal aims to conduct such HRMS based non-target screening of (micro)plastic leachates, including both analyses of reference material and retrospective screening for plastic related chemicals in NORMAN Digital Sample Freezing Platform (DSFP).

The activities planned for 2024 and the expected outcomes are described below.

Activity 1: Compilation of the list of plastic additives, NIAS and their transformation products (TPs)

The NORMAN Suspect List Exchange (SLE) contains suspect lists S46, S47 and S48, which encompass a wide range of plastic additives and associated compounds, allowing to identify and quantify their presence in environmental samples archived in DSFP. Some plastic-related substances are in other SLE lists (e.g. bisphenols (S20) and their alternatives (S67, S97), compounds in plastic toys (S91, S93), etc.). Additional lists are available from e.g. the UNEP report "Chemicals in Plastics", the scientific literature and ongoing studies, often carried out with participation of NORMAN members. As an example, the Joint Nordic Screening Group organised a workshop on 'Chemical additives in plastics as an environmental concern in the Nordic countries' in November 2023. All available lists contributed by the participants will be compiled into a single SLE list of plastic additives, NIAS and their TPs. Information on substances, which are not yet in NORMAN Substance Database, will be generated/compiled. This holds specifically for main fragments in the mass spectra, retention time index (RTI, LC-HRMS), retention index (RI, GC-HRMS), ecotoxicity threshold values (Lowest PNECs), physico-chemical properties and additional hazard data (PBMT, ED, CMR). The information will allow for including the substances in suspect screening list and their follow up risk assessment.

Activity 2: Retrospective screening of selected samples from DSFP

Retrospective screening of ca. 400 environmental samples will be performed using the compiled suspect lists (cf. above). The samples will be representative for both freshwater and marine environment, including water, suspended particulate matter, sediment and biota compartments. Studies in which both NTS with GC- and LC-HRMS were carried out simultaneously with analyses of micro- and macro-litter (as required by the MSFD) will be preferred.

Activity 3: Non-target screening of (micro)plastic leachates

Employing LC- and GC-HRMS, non-target screening analyses will be conducted on leachates from (micro)plastics. From an environmental point of view, leachates are more relevant than the plastic particles themselves as they reflect the transfer of the chemicals to the environment. This approach aims to identify and characterise a broader spectrum of compounds released from plastics, going beyond the predefined suspect lists. Compounds detected in this analysis will be further investigated for their presence in the retrospective screening data (cf. above), establishing a direct link between leachates and environmental samples. The leachates will be prepared by TNO and distributed to all interested participants for analysis by various HRMS techniques. MS/MS spectra of novel additives and NIAS will be contributed to MassBank.

The expected outcome for 2024 include:

- A meeting with all interested members of NORMAN will be organised to kick-off the activity. The scientific plan, engagement of interested laboratories, planning and QA/QC will be discussed and decided;
- Compilation of the suspect list of plastic additives, NIAS and their TPs for the NORMAN SLE;
- Comprehensive identification and semi-quantification of suspected plastic additives, NIAS and their TPs in real world samples archived in DSFP through retrospective screening;
- Discovery of novel contaminants in plastic leachates through non-target screening;
- Integration of datasets on non-target screening of plastic-related chemicals and analysis of micro-litter/macro-litter to improve the understanding of the correlation between the occurrence of (micro)plastics and presence of plastic additives, NIAS and their TPs in the environment;

- Environmental risk assessment of the identified plastic additives, NIAS and their TPs using NORMAN Prioritisation Framework.

CWG-NTS Assessing the spectral quality and diagnostic information of MS2 data acquired with LC-ESI-HRMS

Assessing the spectral quality and diagnostic information of MS2 data acquired with LC-ESI-HRMS (Leader: VU, Frederic Béen, f.m.been@vu.nl and UBA, Tobias Schulze, Tobias.Schulze@uba.de) in collaboration with SU, LCSB, UvA, UFZ, IDAEA-SCIS, NKUA, Eawag and others.

Tandem mass spectra (MS2) are essential for numerous applications, including the curation of spectra libraries and, more recently, the prediction of molecular (sub)structures and potential in-vivo or in-vitro toxicity of detected features. However, the quality of acquired MS2 data can have a large impact on the identification of features and the reliability of predictions. VU and KWR recently developed a machine learning-supported algorithm to automatically assess the quality of MS2 spectra based on a set of mathematical features calculated from MS2 data.

Aim: The goal of this activity is to implement the recently developed algorithm to improve MS2 data from NORMAN members and support their activities. More specifically, we aim to apply the model to data from NORMAN members, including large spectral libraries (e.g., MassBank), refine the model where needed (e.g., quality assessment criteria and model architecture), and finally evaluate its impact on identification rate and MS2-based toxicity prediction (e.g., MS2Tox and MLinvitroTox).

The activities planned for 2024 and the expected outcomes are described below.

Activity 1: Gather MS2 data from NORMAN members and evaluate the model's output versus expert assessment using a quality score. For that we will make use of reference standard mixtures (e.g., NORMAN RTI standard mixture) and circulate them among partners for measurement. Outcome: test the current model on a larger dataset and evaluate whether a scoring system (instead of the current binary output poor vs good) is more useful.

Activity 2: Refine the model where needed based on outcomes from Activity 1 (e.g., input variables, model architecture). Outcome: roll out a more advanced and robust version of the spectral quality assessment model based on Activity 1.

Activity 3: Apply the model on larger datasets, including libraries (e.g., MassBank Europe), actual samples and data processed with different workflows/instruments. Outcome: test the model on real data from different instruments and workflows.

Activity 4: Evaluate the impact of the quality assessment model on the identification rate (e.g., based on spectral similarity scores) and on the outcomes of predictive approaches such as MS2Tox and MLinvitroTox. This can be carried out in parallel to the JPA activity "Integration of computational toxicity driver prioritisation tools to support non-target screening workflows in high-throughput effect-directed analysis" (see "Bringing together NTS and toxicity – Cooperation between DSFP and MLinvitroTox, MS2Tox and other tools).

CWG-NTS & CWG-PS PFAS - Intercomparison study on passive sampling and NTS for PFASs (Phase 2 - follow-up from JPA 2023)

Intercomparison study on passive sampling and NTS for PFASs (Leader: QAEHS k.sarit@uq.edu.au in collaboration with RECETOX branislav.vrana@recetox.muni.cz, NIVA Ian.Allan@niva.no and University of Amsterdam s.samanipour@uva.nl)

This activity was launched in 2022 with the aim to address and identify some of the limitations and opportunities with the passive sampling and broad scale non-target screening (NTS) of PFASs.

Per- and polyfluoroalkyl substances are a large group of compounds that have been used in countless industrial, commercial and manufacturing processes and products for decades. Use and waste disposal of PFASs has resulted in wide-spread environmental contamination. Due to the high stability and mobility PFASs have been detected in in all environmental compartments, as well as in humans. Perfluoroalkyl acid (PFAA) precursors can degrade in the environment to form PFAAs, as well as numerous degradation intermediates. Due to the relatively uncontrolled synthetic routes and environmental degradation pathways, thousands of individual anionic, cationic and zwitterionic PFASs are believed to exist. The vast number and diverse properties of PFASs, and the geographical scale of contamination present enormous analytical and sampling challenges. Current sampling, analysis and identification methods are limited to handful of PFASs including sulfonates, sulfonamides, carboxylates, phosphinates and others. Therefore, NTS is emerging an important tool to characterisation of these compounds and understand their fate in the environment, including degradation and transport processes. Passive sampling is emerging as an important tool for the monitoring and identification of PFASs in waters as they provide *in situ* concentration of samples, in some cases can increase sensitivity and provide a more representative image of PFAS contamination in comparison to grab

sampling due to time-integrative character of sampling. The combination of passive sampling of PFAS and NTS is of high interest for characterising sources and fate of PFAS in the environment and from contaminated source zones. However, inter-laboratory comparisons of the use and interpretation of data with these tools is necessary to increase confidence in their use and application.

Phase 1: Intercomparison of analytical methodologies (2022-2023)

One type of passive sampler was deployed at a highly contaminated sites in Australia along with grab sample collection. The site has wastewater effluent and a diverse range of PFAS sources, selected to represent different matrices and PFAS profiles.

Homogenised passive sampler and grab sample extracts, along with reference standards and blanks were sent to participating laboratories for analysis in Sep/Oct 2023 and results from the laboratories for Phase I are aimed to be submitted by end of January 2024. Report and publication are expected towards Q3-Q4 2024. A total of 27 laboratories from 16countries have received samples for analysis and reporting. In Phase I, the passive samplers, their deployment extraction and analysis and shipping costs were all provided in-kind by QAEHS, UQ.

Phase 2: Intercomparison of passive sampling technologies (2024)

As several different passive sampler configurations for PFAS are emerging, including legacy samplers such as POCIS, Phase II of this JPA would involve co-deployment of several (3-4) different passive samplers at a surface water or wastewater site in the EU. Site selection will represent a range of PFAS sources and profiles.

The aim is to add to data obtained from Phase I of the JPA by additionally examining the (i) how different passive samplers perform for a range of PFAS (ii) examining extraction techniques of each of the labs (as in Phase I the only point of difference examined between the labs is analysis and reporting) and (iii) analysis (i.e. chromatography-mass spectrometry methods). The aim is also to draw conclusions and apply lessons learnt from Phase I in this subsequent phase.

Homogenised passive sampler extracts and passive sampler devices, along with reference standards and blanks will be sent to participating laboratories for analysis. Participants will analyse sampler extracts as well as conduct passive sampler extractions themselves.

We anticipate sampler deployments will be done in EU (coordinated by Recetox) and samplers will be sent to participating labs from there to reduce shipping costs.

Expected outcomes: Sep 2024: Deployment of samplers. Oct 2024: homogeneity test of sample extracts for approximately 10 PFAS using target analysis. Nov 2024: distribution of passive samplers to participants. Jan 2025: Receive data from participants. Results processing and evaluation expected during Q2-Q3 2025.

Workshop on "AI for environmental monitoring and assessment of chemicals and their mixtures"

NORMAN Workshop: AI for environmental monitoring and assessment of chemicals and their mixtures (Leader: UBA, jan.koschorreck@uba.de. UFZ, werner.brack@ufz.de. Eawag, juliane.hollender@eawag.ch and NORMAN Steering Committee)

The transformative potential of Artificial Intelligence (AI) contributes to the achievement of the goals of a green transition in Europe. One example is non-target screening (NTS) and e.g. the characterisation of chemical mixtures in samples from the environment, the derivation of quantitative exposure data, the harmonisation of HRMS data, and the modelling of environmental effects.

A 1.5-day workshop will be organised at UFZ, Leipzig in autumn 2024. The scientific will address the following aspects:

- Gathering perspectives and needs on AI-based methods in environmental monitoring from different stakeholders from policy, authorities, industry and research communities.
- Presenting AI-based use cases in chemical monitoring and assessment from NORMAN partners.
- Discussing the harmonisation of QA/QC metrics to benchmark and evaluate AI-based methods.
- Organising thematic group discussions on AI in environmental monitoring and assessment.
- Initiating an AI strategy for the NORMAN network.

Collaboration of NORMAN in the 5th Joint Danube Survey

Collaboration of NORMAN in the 5th Joint Danube Survey (JDS5) (Leader: EI in coordination with ICPDR)

The JDS5 will take place in 2025. The Danube surveys are organised since 2001 every six years under the lead of the international Commission for the Protection of the Danube River (ICPDR; members 14 European countries and EU). Preparation, implementation and outcomes of the surveys are subject to approval by Water Directors of all involved countries and DG Environment. Further to the successful collaboration of the NORMAN network in the

previous edition (JDS4) it is planned to set up a dedicated Task Group to accompany the preparation of the NORMAN contribution to the monitoring / research activities during the JDS5. A number of collaboration topics have already been identified. The Task Group will contribute to specify in further detail the topics to be promoted and identify interested participants from the NORMAN network.

Interlaboratory studies (ILS) on haloacetic acids and selected pesticides of sulfonylurea compounds

Interlaboratory studies on haloacetic acids and selected pesticides of sulfonylurea compounds (Leader: IWW, Gerhard Schertzinger g.schertzinger@iww-online.de)

There are increasing reports about the occurrence of these substances in the aqueous environment: in surface water, groundwater and for some of them even in drinking water.

Reliable analytical methods are needed to better assess the current situation and to investigate the effectiveness of several measures (such as advanced wastewater treatment) to reduce emission of these substances into surface waters.

However, for these substance groups there are no European or internationally harmonised or standardised analytical methods available so far, and a thorough assessment of the suitability of different analytical methods used is still lacking.

Together with AQS BW, IWW Water Centre will organise interlaboratory studies on these compounds in drinking water.

- The ILS (RV 5/24 TW S11) on the haloacetic acids is scheduled for June 2024. Parameters will be: monochloroacetic acid, dichloroacetic acid, trichloroacetic acid, monobromoacetic acid and dibromoacetic acids;
- The ILS (RV 8/24 TW S5) on selected sulfonylurea compounds is scheduled for September 2024. Parameters will be: amidosulfuron, metsulfuron-methyl, rimsulfuron, thifensulfuron-methyl and triasulfuron.

The studies will combine proficiency testing of laboratories and evaluation of the suitability of methods used.

As a result of this activity a comprehensive report on the outcome of the interlaboratory studies will be delivered with conclusions on:

- the proficiency levels or European analytical laboratories;
- the suitability of analytical methods for analysis of these two compound classes in water samples.

Dissemination of information about the ILS (announcement/invitation, registration form etc.) will be done through the NORMAN website.

Further technical details, registration deadline and the shipment dates can be found at https://www.iswa.uni-stuttgart.de/institute/central-services/lflaqs/aqs/pt/

The proposed budget for this JPA may be revised by the Steering Committee in May 2024. All approved scientific activities will be implemented, independently of the revision of the budget.