February 2022

NORMAN Joint Programme of Activities (JPA 2022)

List of scientific activities organised by the NORMAN network in 2022

We are proud to present the scientific programme which will be promoted by the NORMAN network in 2022.

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 € 265,450, 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 databases.

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.

A summary description of each activity is presented in the following sections.

Contents

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 is at the core of NORMAN activities, providing data and tools to fulfil its goals and visions. The NDS consists of 13 integrated database 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. NORMAN MassBank - 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/ ;
13. Prioritisation - https://www.norman-network.com/nds/prioritisation/.

A new module EMPODAT-SUSPECT (https://www.norman-network.com/nds/suspect/) was developed in 2021 in support of WG-1 and has already been tested on a first dataset of 6.5 million data entries.

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

Automated prioritisation modules in the NDS have been developed for the target substances and suspect substances, following the instructions and guidance from the WG1.

The maintenance of the NDS and its continuous upgrade for new data involves a significant effort. The workplan for 2022 will include:

- Interlinking all NDS modules and quality check of all input data;
- NDS Chemical Occurrence Data (EMPODAT): maintenance, upgrading and feeding of new data into the database; sharing the data with IPCHEM;
- Continuous upgrade of all DCTs for an extended list of NORMAN substances (SusDat), drop-down lists and definitions of obligatory parameters;
- Further upgrade of automated quality control tools for identification/ removal/ flagging of outliers in the collected datasets in EMPODAT;
- Further development of data mining tools to extract raw data from IPCHEM and other database systems and establishment of a workflow for their processing into the 'NORMAN format';
- Enhancement of visualisation and data analysis capabilities of NDS;
- Continuous upgrade and maintenance of SusDat;
- Update of Passive Sampling module with new datasets; design of Passive Sampling – SUSPECT module;
- Upload of new data into the ARBs/ARGs module;
- Upload of new data into the NORMAN SCORE Database - SARS-CoV-2 in sewage (SC2S);
- Upgrade of Substance Factsheets module – systematic collection of all data needed for prioritisation and data download functions;
- WG-2 – Upload of results of bioassay analyses from various projects;
- WG-3 and WG5 – Upload of results from various monitoring projects;
- WG-6 – Upload of data from the ILS on Indoor Environment 2020 – 2021;
- CWG-PS – Upload of data from ILS 2021;
- Collaborative trial NTS in biota - Upload of data from the ILS 2020 – 2021;
- Upload of data from wide-scope target screening and suspect screening of chemicals in top predators and their prey carried out in the LIFE APEX project;
- Upload of data from OSPAR CONNECT and UBA-HELCOM projects.

The setup of a Database Working Group is envisaged, as recommended by the NORMAN Steering Committee.

MassBank Europe and RMassBank

MassBank Europe and RMassBank - Continuous development and upgrade of MassBank Europe and related activities (Activity coordinated by UFZ tobias.schulze@ufz.de **;** LCSB - Luxembourg emma.schymanski@uni.lu; and Eawag, Michele Stravs michael.stravs@eawag.ch in co-operation with Steffen Neumann (IPB Halle) and NFDI4Chem).
In 2022 the continuous development and upgrade of MassBank Europe and RMassBank will be pursued with a focus on:

- Upload of mass spectra to MassBank (UFZ, Eawag, LCSB - all NORMAN members welcome!)
- Maintenance of RMassBank
  - improving input of peak list-based data;
  - integrating mzTAB + MGF input (e.g. as export from pre-processing in other software);
  - integrating JCAMP input and workflow (e.g. Agilent PCDL exported libraries);
  - maintenance and update of existing functions.
- Maintenance of the MassBank server platform
  - maintenance and update of existing functions;
  - implementing a new spectral search function;
  - improving the representation of mass spectra and structures to be more interactive.
- Maintenance of MassBank data
  - maintenance and update of curation functions;
  - integration with PubChem (update annotation, deposition in PubChem, CIDs in MassBank);
  - implementingmore consistent display of chemical identifiers (e.g. preferred MassBank name);
  - a FAIRer presentation of the records (e.g. implement author tags);
  - integration of UOA RTI and ionisation efficiency.
- Fostering and maintaining interoperability with global partners
  - NFDI4Chem, PubChem and others;
  - Integration of MassBank in NFDI4Chem as central repository (2022-2025).
- Prioritisation of chemicals for upload
  - Fostering the discussion on prioritised compounds missing in MassBank (matches to SLE, priority mixtures etc.), create a list of most wanted spectra and establish a platform for exchange of information;
  - Establishment of a chemicals exchange platform to share neat standards for the creation of MassBank records and confirmation of identified compounds;
  - Evaluation of MassBank data regarding 1) chemical space covered and 2) reproducibility of spectra between groups and instrument types.
- Training and demonstration
  - Organising an online workshop on RMassBank processing and downstream analysis using MassBank spectra.

Added value and links with other NORMAN activities and / or other projects:

- Enhancement of non-target identification tools and workflows;
- NORMAN Digital Sample Freezing Platform relies on the fragment information;
- Cross-Action Working Group NTS;
- Interaction with NFDI4chem, PubChem and other global partners;
- Bridging to WG1 Prioritisation.

DSFP upscale - Phase II

DSFP development and upscale - Phase II (Leader: EI alygizakis@ei.sk)

DSFP has proven to be useful for various activities of the NORMAN network, especially the prioritisation of CECs and as an early-warning system for environmental chemical risks. DSFP, as part of the NORMAN Database System (NDS), is a valuable asset for the future activities of the NORMAN network. It is also expected to play an important role in PARC, considering that its functionalities will be expanded to human biomonitoring.

As of September 2021, the platform contained HRMS data from more than 2,500 unique environmental samples around Europe and beyond. The samples covered water (50.02%), biota (22.78%), wastewater (18.81%), sediment (3.98%) and soil (3.11%) matrices.

Several projects have contributed their datasets to the DSFP, including the Joint Danube Survey 4 (JDS4; International Commission for the Protection of the Danube River, 14 European countries and EU; http://www.danubesurvey.org/jds4), Joint Black Sea Surveys (EU/UNDP EMBLAS-II and EMPLAS-Plus projects; http://emblasproject.org), monitoring of Dnieper, Dniester, Siverskyi Donets rivers, Antarctica Station Vernadsky, EU LIFE APEX project dealing with the monitoring of top predators and their prey (https://www.lifeapex.eu), wastewater effluents across Europe and many others. All these HRMS datasets can be revisited to retrieve information about the occurrence of CECs, employing retrospective suspect screening workflow. Semi-quantitative estimates of concentrations of suspects detected in the samples can be obtained and used in the prioritisation process.

The planned upscale involves the creation of a Dataset Management System (DMS), which is a single point of data contribution and administration. Further details are provided in the Factsheet "DSFP Development and upscale - Phase II".

The technical solution was designed in 2021; the DMS and relational database have been set up and the administration and institutional forms have been created (https://dev.norman-data.eu/). The Search API is under construction and it is planned to finalise it together with the open data catalogue and discovery application by June 2022. The project will be tested by beta-testers (UFZ and NILU have already expressed interest); afterwards two revision rounds will follow. After the finalisation, an online webinar will be organised to disseminate the progress and support laboratories in sharing their data.

NORMAN EMPODAT Suspect Database

Update of NORMAN EMPODAT – SUSPECT Database to host suspect screening results in support of prioritisation activities (Leader: EI alygizakis@ei.sk)

The full automatisation of the NORMAN prioritisation scheme is of utmost importance. The 2021 prioritisation exercise of was conducted in an automatic manner for target screening data and in a semi-automatic manner for suspect screening data. This exercise was valuable to provide the needed guidance before the programming of the NTS prioritisation module. To achieve full automatisation, a new NDS module named “EMPODAT – SUSPECT Database” (https://www.norman-network.com/nds/suspect/) was designed and programmed in 2021. This database is able to import the suspect screening results obtained by the DSFP analysis workflow. The proposed activity aims to bring this valuable information to the on-line platform in a harmonised format and make the data available for the NORMAN Prioritisation Framework and any other purposes.

This activity was started in 2021 and additional tasks are planned for 2022:

- Upgrade of the new NDS EMPODAT – SUSPECT module based on the needs of WG1 and NTS CWG
- Retrospective suspect screening on all available DSFP datasets (>2,500) to cover the widest possible spatial, temporal and matrix distribution
- Import of the suspect screening results obtained by DSFP workflow in the EMPODAT - SUSPECT
- Retrieval of information from EMPODAT – SUSPECT to feed the prioritisation module based on the experience from the pilot exercise and DSFP screening output
- Invitation of WG1&NTS CWG experts to rigorously evaluate the prioritisation output and the interfaces.

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).

Better chemical management in line with the goals of the EU Chemicals Strategy and Zero Pollution Action Plan strongly relies on identification and control of pressures through efficient monitoring and knowledge of the properties and use patterns of chemicals. Given the high number of chemicals present in our environment, prioritisation of chemical contaminants is highly demanded by regulators and decision-makers in order to identify and justify priority actions to achieve these goals.

In 2021, the new version of the NORMAN prioritisation framework, combining target and suspect-screening data, was tested on a large-scale case study. A number of tools – IP score, semi-quantified data approach, EMPODAT-Suspect Database, automated prioritisation tool – have been specially created and tested to support the new workflow and enable its integration in the NORMAN Database System (NDS). Further development in the implementation of the new workflow and upgrading of the on-line prioritisation tool are planned in 2022 (Tasks 6, 7 and 8), keeping in mind a possible contribution in support of PARC Task 4.2 (mechanism for identification of priority actions for environmental monitoring, EDC and PFAS campaign) and Task 8.2 (European Early Warning System), EEA indicators for Zero Pollution Action Plan and Green Deal research projects.

In 2022 WG-1 Prioritisation will pursue the work started in the previous JPAs focusing on the following objectives:

Task 1: Support the prioritisation work of the Commission services at European level and comment on relevant documents and queries (WFD Priority Substances, Watch List, PARC, EWS, where relevant) (permanent activity) (INERIS).

Task 2: Collection and compilation of compound-specific information in support of prioritisation (permanent activity) (UBA, EI, Ecotoxcentre).

Pursue the activities started in 2020-2021 to harmonise the existing raw ecotoxicity data to fit the revised NORMAN Ecotoxicology Database metadata requirements; to upgrade the DCT template and transformation tables to fit the new layout, e.g., regarding matrix and asset protection.

Pursue the work relating to the extraction and compilation of additional experimental ecotoxicity data from other existing ecotox databases, i.e. the REACH portal and the UBA ETOX database, (could not be performed in 2021 and will be postponed to 2022).

In 2021, the Ecotoxcentre has adapted its internal templates for data compilation to enable direct transfer of raw data into the NORMAN ECOTOX Database. This has been tested on a set of substances and the corresponding data have already been uploaded to the NORMAN database. This initiative will be pursued in 2022.

Task 3: PNEC derivation activity with the participation of Ecotoxicity experts to derive and approve additional Lowest PNEC values for SusDat compounds, with a specific focus on substances that have been highly prioritised in EU projects using the NORMAN Prioritisation Framework (permanent activity) (UBA).

Task 4 - Integration of a Mixture Risk Indicator as an additional indicator that accounts for the significant contribution of certain mixture components to the total risk - while by themselves not exceeding the PEC/PNEC ratio of 1 (new activity) (UBA).

Task 5: Compilation of data / information regarding 'Use categories' and 'Chemical Functional Use' for the SusDat compounds. The final aim of this activity is to provide a list of 'NORMAN Use categories' and 'Chemical Functional Use categories' and enable substance searches in SusDat by "use" and "functional use" category(ies) (follow-up from 2021) (LCSB, UBA, INERIS, EI).

To achieve this objective, we propose to organise a strategy within WG-1 in line with the ongoing collaboration between NORMAN and PubChem.

Task 6: Prioritisation framework / follow-up activities to apply the new workflow across compartments and specific chemical groups (in 2022, we plan to pursue and publish the analysis of the results of application of NTS workflow on the WW case study. We will address EDCs, PFAS & PMTs in support of PARC and Green Deal projects). (INERIS, EI, UBA).

Task 7: Prepare input to the Early Warning System for Europe (EWS) (link to PARC) (EI).

Task 8: Lessons learnt from the case studies to improve the features of the prioritisation tool (consultation & programming activities). In this task (INERIS, UBA, EI) we will organise a series of meetings (virtual, if possible one physical meeting) for consultation of WG-1 experts on proposals / desk work to revise the features of the prioritisation tool. The programming work is expected to start in 2023 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 by integrating the results of single substance risks at certain sites into a total effect, by mapping the concurrent occurrence of chemical contaminants in Europe, across compartments (UBA, EI, INERIS, UFZ).

It is expected that the activities of WG-1 will help to build fruitful synergies with the work plan of the European PARC partnership currently under construction.

WG-2 Bioassays

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

Task 1: Remobilisation of pollutants during extreme flood events

In this activity NORMAN will organise an international ring study for a comprehensive effect-based and chemical profiling of samples collected during and after the extreme flood event which ravaged several areas of Germany in the summer of 2021.

These events showed the potential effects of climate change, which is expected to render them increasingly severe and frequent. Climate change can interact strongly with other anthropogenic stressors of nature. Thus, a frequently underestimated hazard associated with extreme flood events is the mobilisation or remobilisation of various contaminants. Pollutants released directly into the water from affected and damaged infrastructure as well as pollutants previously bound in sediments and remobilised by the water force during flooding can affect aquatic ecosystems and adjacent terrestrial ecosystems associated with them. The Goethe University was able to collect samples from a number of German locations during the 2021 flooding events.

In this JPA, ten selected sediment and suspended sediment samples collected in the Eifel region in the summer 2021 flood will be tested in a joint ring study. Effect-based methods (EBMs) from the proposed NORMAN / SOLUTIONS battery, additional bioassays on neurotoxicity and chemical analyses will be used to obtain comprehensive insights into the impact of such an extreme flood event in respect of the goals of the Water Framework Directive (WFD).

Generated data will be provided to NORMAN databases and a joint paper will be prepared.

Task 2: 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).

This activity was already proposed in 2021 and a first expert group meeting was held on 29 April 2021. The planned workshop, which could not take place in 2021, will be organised 2022 (resources already allocated in JPA 2021).

The starting point of this task is the already available database developed by Brock et al. (2000a; 2000b) and Van Wijngaarden et al. (2005), in which the effects of chemicals as observed in microcosm and mesocosm experiments were categorised into no effects, slight effects and clear effects using different structural and functional endpoints (e.g. zooplankton, phytoplankton, physico-chemical parameters, macro-invertebrates, fish). This database has been updated till 2009 and is the database behind the PERPEST model which is able to predict the community and ecosystem-level effects of pesticides (Van den Brink et al., 2002). The aims of this task are to update the database, to broaden it (as it currently only contains pesticides) and discuss whether it has the right structure for its use within the NORMAN network.

Rationale: important to include field assessment of ecosystems structure and functioning (aquatic monitoring) as well as semi-field studies performed with emerging chemicals using microcosms and mesocosms. These issues are not addressed in the current WGs.

Task 3: Optimal *in vitro* genotoxicity bioassay testing strategy (Leader: KWR)

The goal is to develop a cost-effective testing strategy by using a minimal number of assays without losing accuracy on the prediction of potential genotoxicity. In 2022 the focus will be on gathering participants, discussing their needs and developing a collaborative proposal for 2023. For that, a meeting will be organised in autumn 2022. Possibilities to align with the Bioactivity Database (see below) will be explored.

Task 4: Follow-up of activities started in 2019 / 2020

The work of WG-2 Bioassays in 2022 will also cover the following ongoing actions from previous JPAs:

- Pursue the development of the **Bioactivity database** (Leader: EI slobodnik@ei.sk, in collaboration with KWR Tessa.Pronk@kwrwater.nl and Miina.Yanagihara@kwrwater.nl; UFZ beate.escher@ufz.de; UBA Peter.VonderOhe@uba.de; and VU timo.hamers@vu.nl). Further to the work done by KWR and VU under JPA2020 (Pronk et al. 2020), the requirements for a NORMAN Bioactivity Database were defined. Resources were allocated on JPA 2021 for: 1) developing and programming the prototype; 2) filling the prototype with data (involving respondents to the questionnaire); 3) testing round of the prototype. In 2021 EI developed a first prototype of the interface of the Bioactivity Database. Actions postponed to 2022: 1) development of the Data Collection Template (DTC); 2) test the DTC on some datasets and 3) define a procedure to derive the potencies of the compounds for each endpoint.

- 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 work, delayed due to COVID-19 crisis, will be pursued in 2022. Expected outcomes, described in detail in JPA 2020, include concrete improvement in fine-tuning different steps such as sample preparation, exposure conditions and final volume of the exposure media for *in vivo* biotesting using standard chemicals. A report and a joint manuscript with recommendations for high-throughput *in vivo* screening in the context of explorative EDA studies will be prepared in 2022.
- CT on **Bioassays for the evaluation of neuroactive and neurotoxic emerging contaminants:** a report (NORMAN internal use) with the results of the ILS has been submitted. A joint manuscript about the outcomes of the study, with a view to the integration of neurotoxicity as an emerging mode of action (MOA) in a battery of EBMs relevant for water quality monitoring, is planned (Leader: Goethe University Frankfurt Hollert@bio.uni-frankfurt.de).
- Peer-reviewed publication on the results of the **NORMAN Genotoxicity ILS** (Leader: KWR Water Research Institute Milou.Dingemans@kwrwater.nl). The manuscript is in preparation.

Task 4: Support the work of the Commission (EBM – CIS WFD Activity) (Leader: Goethe University Frankfurt Hollert@bio.uni-frankfurt.de)

NORMAN WG-2 will continue its activities in support of the EBM – CIS WFD Activity (DG ENV - WG Chemicals), in particular as regards the follow-up actions further to the publication of the EU guidance for use of effect-based tools in the aquatic environment, with a particular focus on the aspects related to the derivation of trigger values to support implementation of effect-based methods in the WFD.

WG-3 Effect-directed analysis - Source-related CECs – Phase II

Working Group N°3: Effect-directed analysis for hazardous pollutant identification (Activity coordinated by UFZ werner.brack@ufz.de and VU marja.lamoree@vu.nl).

Task 1: Contamination patterns, toxicity fingerprints and toxicity drivers of source-related effluents – Phase II (Leader: UFZ werner.brack@ufz.de)

This proposal is the extension of the JPA 2021 study, focusing on the identification of chemical fingerprints and toxicity profiles in different source-related effluents (municipal, industrial, agricultural). The final goal is to: 1) get an overview of possibly relevant sources emitting micropollutants to the water cycle; 2) identify source-related fingerprints and toxicity profiles in WWTP effluents and receiving waters and to characterise and prioritise source-related footprints for management; 3) identify discrepancies between toxicity profiles and identified mixtures in order to prioritise sources for toxicity drivers identification (EDA).

The first stage of this study was performed in 2021, very successfully sampling, extracting and analysing more than 100 samples by 10 NORMAN partners. While chemical fingerprinting will be finalised within the coming months of 2022, toxicity profiling as a basis for future risk driver identification has so far started addressing only a very limited number of samples. The activities in 2022 will include:

- Toxicity profiling: Extensive screening of the chemically characterised source-related samples for a broad scale of endpoints (see Factsheet);
- Mass balance/iceberg modelling to identify discrepancies between observed effects and explainable effects based on extensive chemical screening in order to identify drivers as well as sources with unknown drivers for subsequent EDA;
- WG2/3 workshop on the evaluation of the results of the sources study and for identification of future WG activities.

The project is meant to act as a pilot study to explore source-related approaches in NORMAN in order to enhance the value of monitoring, assessment and prioritisation to management and regulation options. This work will also be embedded in “Project 02” of Task 4.3 of the PARC partnership.

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: 3rd Round NORMAN / QUASIMEME/ EUROqCHARM ILS study on microplastics in environmental samples (Leader: QUASIMEME, Steven Crum steven.crum@wur.nl and NIVA Bert.vanBavel@niva.no in collaboration with Vrije Universiteit Amsterdam, Ike van der Veen ike.vander.veen@vu.nl)

The first two rounds (JPA 2020 and 2021) have confirmed that there is still a large variance between the results of different laboratories using different methods. The current 'state of the art' with interlaboratory variation as high as 100% for sediment and biota (fish) samples is not satisfactory for large scale monitoring.

Activities in 2022 will be devoted to organisation of the third round of the ILS for the analysis of microplastics in environmental samples in collaboration with QUASIMEME and EUROqCHARM. The third round will include standard tablets containing a known amount of a mix of different plastic polymers, a sediment sludge and a biota sample with a mix of different polymers added. Suggested methods based on flow diagrams of the most used protocols will be made available to take harmonisation one step further to improve the comparability between the participating laboratories.

A workshop will be organised in September 2022 in Amsterdam at the VU-University to evaluate the results of the ILS and harmonise methods and reporting formats.

WG4 will coordinate collaboration between several ILS initiatives organised during the period 2022-2024 by different EU projects (EUROqCHARM, Labplas, PlasticTrace) and other initiatives (JRC/BAM/UBA and ISO/CEN) in which several NORMAN members participate.

More info:

https://science.vu.nl/en/research/environment-and-health/projects/microplastics-ws-and-ils/index.aspx.

Task 2: Follow-up of activities started in 2021

The work of WG-4 in 2022 will also cover the following ongoing actions from previous JPAs:

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

  Several small MPs (< 10 µm) of the most commonly used polymer types (polyethylene (PE), polypropylene (PP), polyamide or nylon (PA), polyethylene terephthalate (PET), PS (polystyrene) and PVC (polyvinylchloride) were produced in 2021 by mechanical fragmentation at NIVA and further separated into nano-size fractions. These fractions will be characterised by dynamic light scattering techniques (particle size distribution and surface charge), resistive pulse sensing (particle size distribution) and electron microscopy (shape of the particles) at EAWAG in the beginning of 2022 and two suitable polymers will be selected for the production of a reference material at NIVA in the form of dissolvable soda tablets and submitted to strict QA/QC procedures.

  The environmental monitoring of plastics is high on the agenda of countries and international organisations worldwide. Large scale national and regional monitoring programmes are, however, hampered by the lack of reference materials for QA/QC and standardisation of methods. There is great variation in the quality and comparability of data on the presence of plastics in the environment. Robust and validated harmonised methods and QA/QC tools are still not in place. To select candidate reference materials and produce size fraction is a major challenge. Currently no reference materials of micro-plastics (<10 µm) and nano-plastics (< 1 µm) are available. This activity addresses the development of small sized micro- and nano-polymer reference materials.

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).

Task 1: Upgrade of the Antibiotic Resistance Bacteria and Genes Database: The database (https://www.norman-network.com/nds/bacteria/index.php) was designed on the basis of the data-collection templates (DCTs) created in the ANSWER project. In 2022 we plan to upgrade the database to support chemical data on antibiotics and their transformation products as well as antimicrobial substances. Moreover, the DB will be enriched with advanced visualisation options. The data that will be contributed is expected to establish baseline concentration levels in WW intended for reuse and in other matrices. Preparation of a manuscript (see Factsheet).

Task 2: Population of the SARS-CoV-2 in sewage (SC2S) Database (NORMAN SCORE): in 2021, the SC2S database was populated with 556 data sets from 10 countries. An article co-authored by 59 contributors was published as a Water Research Making Waves article in April 2021 (https://doi.org/10.1016/j.watres.2021.117167). In 2022 the focus will be on working with volunteers who can commit to the monthly submission of data from their local WWTPs, enabling a longitudinal data set of WW characteristics, SARS-CoV-2 and case numbers to be developed for as many counties/locations as possible. After a period of one year the data will be evaluated to explore relationships between parameters (see Factsheet). A short report will be prepared and – if data permits – a research paper.

Task 3: Upgrade of NORMAN Databases for CECs in reused matrices: The risks linked to chemicals in reused matrices such as water and sewage sludge are mostly unknown. Moreover, occurrence data and quality targets (or

threshold values) are needed to characterise and prioritise those risks. WG5 have identified as a new priority the collection and dissemination of such data to support research projects, policy makers and environmental managers. This initiative is supported by the Water Europe association. Further to the WG-5 survey performed in 2021, activities planned for 2022 will focus on the upgrade of NORMAN DB (DCTs and SEARCH functions of EMPODAT and ECOTOX) to allow integration of new data on occurrence and quality targets related to reuse practices, including reclaimed water, stormwater, sewage sludge, sediment and soil. A pilot study will be performed to test the practicality of the modified DCTs for regular submission of data from volunteers of NORMAN and Water Europe.

Further collaborative initiatives are possible according to the mandate approved by the WG https://www.norman-network.net/?q=node/142.

Links with all the other WGs and in particular the newly set up Terrestrial Environment WG and the Prioritisation WG are envisaged.

WG-6 CECs in the indoor environment

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

Task 1: Expanding the scope of the WG to also cover ambient/outdoor air

- (see 'Expanding the scope of WG-6 to outdoor air')

Task 2: CT on Passive air sampling and wide-scope suspect/non-target screening for organic substances in indoor and outdoor air (in collaboration with PS-CWG)

- (see 'CT Passive air sampling and NTS indoor and outdoor air').

Task 3: Follow-up of activities started in JPA 2019/2020/2021

WG-6 will focus on finalising the ongoing activities:

- **2nd CT on non-target and suspect screening methods for organic substances in European indoor dust**: Data analysis started in autumn 2021 and will be finalised in 2022. A meeting to present and discuss the results will be organised in spring 2022. Report/scientific publication is planned for autumn 2022 (Action leader: peter.haglund@chem.umu.se Umeå University)
- **Geographical distribution of organic substances in European indoor dust**: A meeting will be held in February 2022 with labs that have volunteered for analysis, to discuss and agree on chemicals to be analysed and extraction protocol. Dust samples will then be extracted by Umeå University and extracts will be sent out before April 2022. Deadline for data reporting (after summer 2022, exact date to be decided). (Action leader: peter.haglund@chem.umu.se Umeå University)
- **Intercomparison study of dust sampling methods**: In 2021, two datasets have been finalised – chlorinated paraffins and POPs. Data analysis will be finalised early 2022. The WG will try to gather data also on other compounds (plasticisers and flame retardants). A report including recommendations on sampling strategies for CPs and POPs (early 2022) to be expanded with plasticisers and OPFRs will be finalised in pring 2022. Scientific publication in autumn 2022 (Action leader: pim.leonards@vu.nl VU).
- **Collection and uploading of indoor data in NORMAN Indoor Environment database**. JPA 2021 activity postponed to 2022, including allocated budget (Action leader: EI alygizakis@ei.sk).

WG-6 Expanding the scope to ambient air

WG-6 - Expanding the scope of WG6 to outdoor air (Activity coordinated by Stockholm University jon.martin@aces.su.se, NILU Pernilla.Bohlin.Nizzetto@nilu.no in collaboration with Aarhus University Katrin Vorkamp kvo@envs.au.dk, RECETOX, lisa.melymuk@recetox.muni.cz and VU pim.leonards@vu.nl)

WG-6 proposes to expand the main objectives of the WG to include outdoor air. This will entail amendments to name and original objectives of the WG.

In 2022, WG-6 will initiate this process by:

- Inventorying established infrastructures and monitoring networks for ambient air in Europe– what and how do they measure, where do they store the data – making sure that NORMAN complements and does not duplicate (NILU, RECETOX, AU);
- Expanding the data collection template (DCT) and NORMAN database for ambient air;
- Organising a workshop with established networks and PARC (June or September 2022) (SU, AU, NILU);

- Defining how and what NORMAN (WG-6) can do, or needs to do, to incorporate outdoor air in the WG6 objectives and activities with the ultimate goal to enable an international early-warning system for emerging airborne substances.

Added value: Air is an important matrix for transport, distribution and exposure processes. Air is the fastest and most efficient way for volatile and semi-volatile compounds, incl. most POPs, to travel into the Arctic and other remote areas. Air represents an important vector for aquatic and terrestrial food-chains. Moreover, even some high priority organic chemicals mainly transported with water, such as the per- and poly-fluoroalkyl substances (PFAS) and emerging persistent mobile organic contaminants (PMOCs), have major airborne sources. Air is a priority matrix for the Global Monitoring Plan of the Stockholm Convention, thus having an important indicator function for the regulatory effectiveness. There is a close link between outdoor air and indoor environments, as the sampling methodologies are similar, indoor air is both a source to and receptor of ambient air, thus detectable substances are common to both matrices. Important research questions, such as the gas-particle partitioning in air, are still not fully understood. Regional air monitoring networks (e.g. EMEP, MONET, AMAP), as well as monitoring activities at national level and international levels often focus on legacy pollutants although air monitoring, due to its quick reaction to changing sources and environmental conditions, offers important functions for an Early Warning System, including the identification of emerging airborne substances.

Recent development of new air sampling adsorbents (e.g. PDMS-based and ABN adsorbent) are now enabling a broadening of the chemical window for air monitoring, as these adsorbents are relatively clean and stable and do not require destructive and selective clean-up methods. This makes them, suitable for wide-scope suspect and non-target screening analyses, and perhaps even for toxicological testing.

WG-7 CECs in soil and terrestrial environment

Working Group N°7: CECs in the terrestrial environment (Activity coordinated by NILU Linda Hanssen lha@nilu.no and UBA Annegret.Biegel-Engler@uba.de)

The terrestrial environment deserves greater attention in the overall assessment of CECs and chemical risks. It is acknowledged that significant knowledge gaps exist about the occurrence levels, bioaccumulation and risks of CECs in terrestrial ecosystems. Further to the conclusions of the GA meeting 2019, where the topic of CECs in the terrestrial environment – research & monitoring activities in support of EU policies and soil-related SDGs – was proposed for discussion, it was decided that an action at the level of the NORMAN community would be justified to address more systematically existing knowledge gaps in the terrestrial environment.

A survey among the NORMAN members was organised in 2020 and a workshop took place early in 2021 to share results of key EU-wide activities, discuss common goals and develop a roadmap for the WG.

The following actions will be organised as part of WG-7 in 2022:

Task 1: Analytical case study for ESB soil samples to identify ubiquitous compounds

- see ‘ESB soil samples to identify ubiquitous compounds’

Task 2: CECs in soil and terrestrial organisms from different trophic levels

- see ‘CECs in terrestrial organisms from different trophic levels’

WG-7 Environmental Specimen Bank: soil samples to identify ubiquitous compounds

WG-7: Analytical case study for ESB soil samples to identify ubiquitous compounds (Activity coordinated by UBA Annegret.Biegel-Engler@uba.de)

The German Environmental Specimen Bank (ESB) offers soil samples from different ecosystem types (urban, forestry, agrarian and semi pristine) in 9 sampling regions since 2002, see www.umweltprobenbank.de/en .

The samples have been collected according to standardised protocols and they are archived at ultra-low temperatures (<-150°C) to preserve their biological and chemical integrity. So far, temporal and spatial data have been gathered for specific compound groups, including legacy OCPs, PFAS, chlorinated paraffins, brominated and chlorinated flame retardants. They are also being studied using genetic methods, such as eDNA metabarcoding, to provide information on temporal changes in biodiversity.

It is planned to make UBA funds available to support interested laboratories for analysis of these specimens to identify contaminants that are ubiquitous or that are associated with specific ecosystem types and land uses.

Added value: Not much is known about chemicals in soil so far. National screenings often include only a small number of compounds, such as heavy metals. However, many chemicals are transferred to soil via air, application of fertilisers,

biosolids, etc. It is important to start to advance our knowledge concerning chemical contaminants in soil and try to find out which substances we have overlooked so far.

WG-7 CECs in terrestrial organisms from different trophic levels

WG-7: CECs in terrestrial organisms from different trophic levels (Leader: NKUA, Nikolaos Thomaidis ntho@chem.uoa.gr in collaboration with EI slobodnik@ei.sk, INERIS valeria.dulio@ineris.fr, OFR olivier.crouzet@ofb.gouv.fr and olivier.cardoso@ofb.gouv.fr, UBA jan.koschorreck@uba.de))

The proposed activities aim to reduce knowledge gaps and investigate the presence of CECs in terrestrial biota specimens. The study will be performed in close collaboration with the new NORMAN WG on Soil and terrestrial environment. In particular, the WG on Soil and the terrestrial environment will be used as an opportunity to obtain expert advice on the monitoring strategy and the various activities of the study.

Planned tasks (2022 - 2023) include:

- Review of sample preparation protocols and analytical strategies for the determination of CECs in soil and terrestrial biota samples
- Critical review on the profile of CECs detected in different matrices (soil, liver, muscle tissue, eggs, feathers, blood and feces)
- Investigation of potential bioaccumulation in the upper trophic levels of the terrestrial food chain
- Comparison of CECs detected in aquatic versus terrestrial biota samples based on their physicochemical properties
- Collection of ca. 10 samples from a European country representing various trophic levels (e.g. worms, birds of prey, raptors) and their analysis by wide-scope target (>2,200 CECs), suspect (>65,000 CECs), and non-target screening methodologies. The design of the study will be defined in consultation with the experts of the WG-7 on "CECs in Soil and Terrestrial environment"
- Collection of different matrices of analysis (ca. 4 samples) from the same specimen of a raptor (such as liver, muscle tissue, feathers, blood) and analysis by wide-scope target (>2,200 CECs), suspect (>65,000 CECs) and non-target screening methodologies
- Publication on analytical methodologies for the presence of CECs in terrestrial biota samples

This collaborative activity is connected with the EU funded LIFE APEX program (LIFE17 ENV/SK/000355), coordinated by EI, and provides an opportunity to link with the start-up phase of the WG on CECs in Soil and the Terrestrial Environment.

WG-8 Marine environment

Working Group N°8: Marine environment (Leader: EI slobodnik@ei.sk in collaboration with Marine Institute, NIVA, NILU, UBA)

Several large-scale marine environment specific projects were carried out in past years which demonstrated the feasibility of the use of many NORMAN-developed tools in support of the implementation of the Marine Strategy Framework Directive (MSFD), including NTS, passive sampling, prioritisation, setting up marine ecotoxicity threshold values and monitoring of microplastics.

The creation of WG-8 on Marine environment has been proposed and approved in 2021.

The kick-off meeting could not take place in 2021 and was postponed to February-March 2022.

A number of activities have been proposed and will be discussed at the kick-off meeting as a basis for the WG roadmap:

Task 1: Organisation of the kick-off meeting

Task 2: Systematic sharing of published and proposed marine biota, water and sediment ecotoxicity threshold values for inclusion in the NORMAN Ecotoxicology Database (EI, UBA, all)

Task 3: Sharing of existing passive sampling data (NIVA, RECETOX, Marine Institute, all)

Task 4: Sharing of wide-scope target and suspect screening data (all)

Task 5: Prioritisation of marine specific CECs in European sea water, biota and sediments using (updated for NTS) NORMAN Prioritisation Framework (EI, INERIS, UBA, all)

Task 6: Chemicals in polar regions (NKUA, EI, UBA, NILU, NIVA, all)

Task 7: Microplastics (NIVA, all)

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).

The following actions will be carried out as part of the CWG-NTS Activity in 2022:

- NORMAN Suspect Lists Exchange and associated "SusDat" database: Database development and maintenance (EI, UoA and LCSB,) (see "Suspect List Exchange and SusDat");
- MassBank Europe - Continuous development and upgrade (UFZ, LCSB, Eawag and IPB Halle) (see "MassBank Europe");
- Digital Sample Freezing Platform upgrading (EI) (see "Databases – NORMAN DSFP");
- Update of EMPODAT – SUSPECT database - a new NDS module to host suspect screening results (EI) (see "NORMAN EMPODAT – SUSPECT");
- NORMAN CT on Passive air sampling and wide-scope, suspect and non-target screening for organic substances in indoor and outdoor air (SU / NILU / AU / NIVA / INRAE);
- NORMAN CT on passive sampling and suspect and non-target screening for PFASs (QAEHS / RECETOX / VU);
- PFAS suspect HRMS lists and lists of PFAS-containing products (QAEHS / CNR-IRSA, University of Amsterdam);
- Workshop NTS - Analytical fundamentals – Data analysis – Implementation (KU) (see AW-1). The workshop was postponed to 2022.

Follow-up of activities started in JPA 2019/2020/2021 (these activities, started in 2019/2020/2021, were delayed due to COVID-19 crisis and connected issues. NORMAN members can find the results so far available and plans for 2022 in the slides of the virtual CWG-NTS meeting of 16 September 2021 - http://www.norman-network.net/?q=node/384:

- **Collaborative trial on (semi-)quantitative non-targeted analysis with LC/ESI/HRMS** (Stockholm University and NKUA) (see "CT NTS semi-quantification" JPA 2020); In October 2021, nine water samples were sent to 46 laboratories around the world. Workplan for 2022: 1) Data curation. 2) Data analysis: comparison of the semi-quantification accuracy across methods, chemicals, instrument types, and analysis methods. 3) Creation of an interactive dashboard for easy access to the results. 4) Writing a publication, coordinating input from participating labs. 5) Uploading data in DSFP and integration of the most precise approaches to DSFP and NDS;
- **NORMAN Non-target screening guidance paper** (UFZ) (see "NTS Guidance document" JPA 2020); a draft version is under discussion publication in a peer-reviewed journal is expected by end of 2022;
- **Development of the NORMAN GC-HRMS workflows** (NKUA, NILU) (see "NORMAN GC-HRMS workflows" JPA 2020) prioritisation of GC-amenable compounds, purchasing, distribution and finally acquisition of reference standards is ongoing. A reproducible prioritisation of GC compounds based on real occurrence data was achieved. The prioritised substances were supplemented with additional substances based on the literature. Acquisition and distribution of reference standards is ongoing. GC functionality for DSFP was programmed and successfully tested. Further validation will be achieved using the data from the reference standards by the participating laboratories;
- **Interpretation of data from the ILS coupling a passive sampling approach with non-target screening.** The datasets were published in an open access "Data Note" DOI: 10.1038/s41597-021-01002-w and data interpretation is ongoing jointly by some groups (NIVA and INRAE). Further project proposals for data treatment will come in 2023;
- **2nd round of the NORMAN Network Early Warning System** initiative (**NormaNEWS2**) (NIVA, NKUA) (see "NormaNEWS2" JPA 2020); all participants have submitted their data, data quality assurance and assessment are ongoing (2021-2022);
- **ILS on suspect and non-target screening in biota**: All data have been submitted and preliminary data evaluation presented by SLU at a virtual workshop in August 2021. Further data evaluation and publication is planned for 2022 (manuscript already circulated among the co-authors);
- Explore the current **application domain of NTS methodologies**, aiming to specifically address the existing gaps on highly hydrophilic contaminants and hydrophobic compounds (see "Expanding and validating the chemical domain of current NTS methodologies"); application domain already added as a new field in SusDat; a paper is in preparation;
- **Target / suspect screening of indoor dust samples to investigate the geographical distribution** of organic substances in European indoor dust (see "WG-6 Task 1" JPA 2021); work in progress;
- **ILS on non-target screening and suspect screening methods for organic substances in European indoor dust** (Umeå University) (see "WG-6 Task 1" JPA 2021); work in progress.

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).

Task 1: 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)

The combination of passive sampling of PFAS and NTS is of great interest for characterising sources and fate of PFAS in the environment and from contaminated source zones. However, interlaboratory comparisons of the use and interpretation of data with these tools is necessary to increase confidence in their use and application.

This activity will aim to address and identify some of the limitations and opportunities with the passive sampling and broad scale NTS analysis of PFASs.

We propose to deploy one or two types of passive samplers at a highly contaminated site over two weeks. The site proposed will be a surface water site such as a river or lake system and would include a diverse range of PFAS sources.

Passive samplers that have been deployed (including at least a Microporous Polyethylene Tubes (MPT) passive sampler for PFAS sampling as well as a second sampler configuration of interest to the group, (e.g. POCIS or o-DGT)) will be sent to participants along with sample extracts. These will all be provided and shipped by QAEHS to interested laboratories for extraction and analysis of samplers and/or extracts. Participating laboratories will analyse the samples using their in-house techniques (or recommended methods) and report semi-quantitative and suspect screening results back to the organisers.

The aim will be to examine (i) different extraction techniques between laboratories (ii) analysis (i.e. chromatography methods) and (iii) processing methods for these compounds. The trial will aim to investigate and compare a subset of target PFAS, as well as the identification and reporting of suspect PFAS lists via NTA. It is anticipated that data will help with understanding the performance, reproducibility and robustness of PS and NTS methods identified through this process and help guide the process towards the use of these tools in compliance and risk assessment frameworks.

Expected outcomes for 2022: initialise and launch the activity by June 2022, distribute samples / extracts to participating laboratories by August 2022. Collect data by December 2022. Data processing and evaluation will be carried out in 2023.

Task 2: One-stop shop for passive sampling (Marine Institute / Dublin City University)

Recent years have seen increased research and monitoring interest in the application of passive sampling techniques for the measurement of pollutant levels in the aquatic environment. While there is keen interest in various passive sampling methodologies, individual research institutes and monitoring agencies often work on one-off or specific projects independent of similar initiatives taking place within the research community. As a consequence, much of the monitoring and research data can remain hidden within the 'grey' literature and thus can either be lost or underutilised in supporting the applicability of passive sampling as a monitoring tool.

This initiative seeks to develop a 'one-stop shop' approach to collate relevant passive sampling study information into a central repository. It is proposed that a reporting template be developed that would not overly focus on collation of analytical data itself but more so on key validation / modelling Information underpinning these studies (e.g. scope of analysis, robustness, influence of biofouling, Kp_W etc) for a wide range of passive sampling techniques. This information is fundamental to supporting PS as a monitoring tool/matrix. Critically it is proposed to then try to collate similar performance characteristics for both biota and water sampling techniques. When integrated with the passive sampling data, it is proposed to then critically evaluate passive sampling as a monitoring technique, in parallel with the more conventional spot water and/or biota techniques. In addition to this being a useful resource collating these data, it is envisaged that research gaps can then be identified through this process.

The main actions planned for 2022 will be:

- Circulate a memo to NORMAN members explaining the rationale and to request support for the activity (March 2022);
- Generate a sharepoint type portal to collate key published and grey literature provided by members;
- Develop a listing of key performance characteristics that underpin different methods of passive sampling compared to biota and/or water analysis (e.g. from ease of sampling through to detection limits and cost benefits) (May 2022);
- Develop a simple easy-to-use template to collate performance characteristics reported in key literature;
- Meeting of all interested members to develop the template and further promote the activity (Sept 2022);
- Complete a first draft project report (Dec 2022).

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);
- Workshop on PS for substances with EQS_{water} in support of chemical monitoring for the WFD - the workshop has been postponed to spring 2022 (ongoing);
- Interpretation of data from the interlaboratory study coupling passive sampling approach with non-target screening. The datasets were published in an open access "Data Note" DOI: 10.1038/s41597-021-01002-w and data interpretation is ongoing jointly by some groups (NIVA and INRAE). Further project proposals for data treatment will be made in 2023.

CWG-NTS: NORMAN Suspect List Exchange (SLE) and Substance Database (SusDat)

NORMAN Suspect List Exchange (Leader: LCSB, Luxembourg emma.schymanski@uni.lu) and **SusDat** (Leader: EI slobodnik@ei.sk and Nikiforos Alygizakis alygizakis@ei.sk in collaboration with NKUA Nikolaos Thomaidis ntho@chem.uoa.gr and Reza Aalizadeh raalizadeh@chem.uoa.gr)

This activity involves the addition of new lists to the Suspect List Exchange, which can then feed into SusDat, which has become the chemical database behind all NORMAN databases.

As NORMAN-SLE is gaining increasing attention as an expert knowledge base with high potential for greater impact, some additional resources are again requested this year to help curate and add necessary lists already identified as critical gaps (increase coverage, including transformation products) and also work towards a more sustainable model following FAIR principles and allowing direct and automated (as far possible) integration into international resources.

Activities to be pursued in 2022:

- Website maintenance and development;
- Addition of new lists from external contributors when they become available;
- Addition of new lists strategically selected to fill identified knowledge gaps;
- Addition of lists to specifically save/register/link transformation product information;
- Archiving of all datasets on Zenodo (https://zenodo.org/communities/norman-sle);
- Deposition of all substances in PubChem;
- Progressive addition of annotation content to PubChem to fill information gaps;
- Extension and development of Transformations functionality with PubChem, both in terms of datasets and integration into workflows;
- Integration of lists into PubChem and CompTox Chemicals Dashboard;
- Development of new strategies to deal with UVCBs;
- Further development of strategies to deal with tentative/unknown/related structures;
- Publication(s) on ideas and methods behind Suspect List Exchange;
- Open software/packages/approaches for curation/merging once appropriate.

Maintenance and improvement of NORMAN Substance Database (SusDat) (EI slobodnik@ei.sk and alygizakis@ei.sk)

SusDat is one of the core modules in the NDS (most visited module in 2021) together with SLE. The objective of this task is to continue with (i) systematic upload of individual substance lists contained in the Suspect List Exchange (SLE), (ii) their merging and chemical curation, and (iii) adding missing and new information.

Actions to be pursued in 2022:

- Addition of *in silico* predicted Retention Time Index (RTI) values for electrospray ionisation (both positive and negative) and P-PNECs for all substances in SusDat;
- Update of RTIs and P-PNECs for substances with updated chemical structure;
- Application of an automated curation workflow developed in previous years to update the validation level for all substances;
- Adding validation level information for newly added substances;
- Addition of qualifier fragment ions;
- Addition of critical chemical identifiers;
- Addition of preferable analytical methods for each compound (i.e. GC-EI, LC-(+/-)ESI etc.);
- Investigation of potential deployment of the automated curation workflow;
- Addition of toxicity threshold data for terrestrial environment and human health;
- Addition of consensus models for logBCF, logKoa, logKoc and logKow;
- Addition of ionisation efficiency (logIE) values.

Collaborative Trial Passive air sampling and NTS indoor and outdoor air

WG-6 / CWG-PS / CWG-NTS: NORMAN CT on Passive air sampling and wide-scope, suspect and non-target screening for organic substances in indoor and outdoor air, jointly organised by WG-6 (Stockholm University jon.martin@aces.su.se, NILU Pernilla.Bohlin.Nizzetto@nilu.no Aarhus University Katrin Vorkamp kvo@envs.au.dk) and CWG-PS (NIVA Ian.Allan@niva.no and INRAE cecile.miege@inrae.fr)

Activities in 2022 will focus on:

- invitation of participants (end of March);
- preparatory workshop (back-to-back with an existing meeting in Europe) to discuss and plan the sampling strategies (number of samples), sample preparation, data acquisition, data processing and data interpretation;
- conducting air sampling by preparing sampling adsorbents and deploying samplers (autumn 2022). It is suggested to use one type of adsorbent, deploy it in two locations (indoor and outdoor), and test two exposure times (2 weeks and 4 weeks). The use of indoor environments will allow comparison of results from the CT on indoor dust from homes and public environments in Europe (WG-6).

The activity will be pursued in 2023 (i.e. extract the samplers and distribute the extracts; data collection and evaluation; preparation of a scientific paper).

Added value: Until now it has been a challenge to apply NTS for air sample analysis, partly because the commonly used air sampling adsorbents cause major interference and often require destructive or very selective clean-up processes that narrow the screening to only very persistent substances. Very recent developments of new air sampling adsorbents may finally enable the application of NTS to air samples, both from indoor and outdoor environments. Yet very few laboratories have applied NTS on air samples to date.

Another challenge is NTS data comparability. The experiences from previous collaborative trials (CTs) involving NTS of indoor dust samples (both GC-MS and LC-MS) under WG-6, as well as other NORMAN CTs on NTS, have shown that the overlap and agreement between NTS laboratories is still poor. Further effort is needed in intercomparison studies and development of harmonised procedures if we want to extend the application of NTS techniques from research to regulatory monitoring initiatives. Here, a combination of testing the new passive air sampling adsorbent in a few locations and NTS analyses of a broad group of participating laboratories is expected to help the community to take important steps forward towards improved harmonisation of practices and data comparability.

Workshop NTS - Analytical fundamentals – Data analysis – Implementation

CWG-NTS: Workshop Non-target screening Analytical fundamentals – Data analysis – Implementation (Leader: University of Copenhagen, Giorgio Tomasi gito@plen.ku.dk , Jan H Christensen jch@plen.ku.dk).

This two-day workshop will take place in week 48 (28th Nov. – 2nd Dec) in 2022 in Odense. The first day will be dedicated to next generation analytical platforms for NTS, e.g., HILIC, SFC, ion mobility, 2D GC-MS and 2D LC-MS, and related data workflows. The second day will show examples of implementation in regulation and industry with emphasis on successes and obstacles related to scale and outside-academia operationalisation.

The Danish scene currently features a strong collaboration between industry, regulators and academia, which favours implementation, marketing and widespread take-up of non-target technologies. For instance, University of Copenhagen initiated the GANDALF and VANDALF Innovation Fund Grand Solutions Projects in collaboration with industry leaders and regulatory bodies such as Eurofins A/S and the Danish EPA for implementation of non-target approaches in soil and wastewater assessment.

The workshop would link to several NORMAN WGs, the NTS cross-working group, but also WGs 1, 3 and 5. It would be an excellent opportunity to present to the industry the work which was done e.g. on the data bases, and on prioritisation.

It is envisaged to organise the workshop back-to-back with NORMAN GA meeting (hosted at Danish EPA in Odense).

PFAS suspect HRMS lists and PFAS-containing products

CWG-NTS: PFAS suspect HRMS lists and lists of PFAS-containing products (Leader: University of Queensland, Pradeep Dewapriya p.dewapriya@uq.edu.au and Sarit Kaserzon k.sarit@uq.edu.au in collaboration with CNR-IRSA sara.valsecchi@irsa.cnr.it and University of Amsterdam Saer Samanipour s.samanipour@uva.nl)

With this activity we aim to firstly (Task 1) consolidate available PFAS suspect lists, curated data including PFAS MS/MS libraries and information on PFAS-containing products. This task will start with the consolidated list of PFAS lists in NORMAN SLE and will expand the information and resources in that list to improve the identification confidence of PFAS in suspect screening. This information will then be used to analyse, identify and report different PFASs in products and contaminated matrices (Task 2).

The types of samples and products that will be considered in Task 2 will be defined at the initiation phase of the JPA and input will be sought from the other participating organisations.

Ideally, a broad range of PFAS-containing consumer and industrial products and contaminated matrices (i.e. textiles, food packaging) will be analysed on HRMS by participating laboratories and screened using NTS suspect screening approaches and workflows and the consolidated library. Data files will be exchanged among the labs to examine the interlaboratory performance of identifying the PFAS. The knowledge and expertise of PFAS identification and reporting will be shared among laboratories and is expected to contribute to shaping and consolidating the reporting of PFAS using HRMS methods for better harmonisation and confidence.

The workplan for 2022/2023 includes:

Task 1: Consolidating PFAS lists in NORMAN SLE and curated HRMS data (Jan-Dec 2022)

- Joint activity kick-off meeting and finalising proposed work plan – March/April 2022
- Knowledge exchange workshop and recruiting participants for HRMS data submission and interlaboratory assessment tasks
- Literature survey on PFAS-containing products, PFAS suspect lists and HRMS libraries
- Consolidating PFAS suspect list and HRMS information
- Workshop/meeting on consolidated Suspect List results and PFAS-in-products literature results. Discuss plan for Task 2; Product suspect screening – Dec 2022

Task 2: Product suspect screening and interlaboratory exchange (Dec 2022 – Dec 2023)

- Based on agreement and consolidation in the Dec 2022 workshop – we will invite submissions from laboratories and agree on (i) the analytical methods and workflows for screening PFAS in products (ii) the products that will be screened (iii) the data repository to share HRMS data (iv) and the reporting template (Dec 2022)
- Participating laboratories to submit HRMS data and their results from suspect screening workflows to a repository - for interlaboratory data screening comparisons (March 2023)
- Submitted data will be (i) assessed for compatibility between laboratories' identifications and reporting and (ii) `used to investigate the identification and occurrence of PFAS in selected consumer products (Nov/Dec 2023)
- Organisation of a workshop to communicate the outcome and preparation of joint publication – Dec 2023

PFAS analytical exchange - TOP Assay Method Comparison

Per- and polyfluoroalkyl substances (PFAS) TOP Assay Method Comparison – Desk based laboratory questionnaire and report (Leader: Environment Agency England alun.james@environment-agency.gov.uk)

Although the TOP assay is now an established technique offered by a range of accredited commercial laboratories, the methods used by laboratories can vary and the oxidative reaction mechanism and pathway are not fully understood.

Results from the NORMAN PFAS analytical exchange questionnaire (JPA 2021) indicates that ~23% (cohort of 57) of laboratories routinely undertake TOP assay analysis with a further 14% outlining this as a future development priority. The aim of this activity is to further the work undertaken in JPA 2021 to better understand the current methods being employed and the reasoning / barriers for selecting the method.

The outcomes of this study can be used to shape future method adoption and encourage consistency to detect and measure PFAS in the environment.

The workplan for 2022 includes:

- Targeted questionnaire on TOP assays across the network and beyond (May-Sep 2022)

- Data analysis (Oct-Nov 2022)
- Virtual workshop (Nov-Dec/GA 2022)
- Report (Feb/March 2023).

PFAS Workshop

NORMAN Workshop: Monitoring PFAS in support of the EU Chemical Strategy for a PFAS-free environment (Leader: NILU, martin.schlabach@nilu.no, Vladimir Nikiforov van@nilu.no, Pawel Rostowski pawel.rostkowski@nilu.no ; Norwegian EPA audun.heggelund@miljodir.no ; KWR Frederic.Been@kwrwater.nl; Aarhus University, Katrin Vikram kvo@envs.au.dk and NORMAN Steering Committee)

Organisation of a 1.5-days interdisciplinary workshop (Brussels, June 2022) to discuss NORMAN contribution to PFAS EU policy (with a specific focus on PARC):

- Monitoring PFAS across compartments and legislation;
- Using state-of-the-art methods (target, sum parameters, NTS, effect-based methods);
- In support of better chemical managements, circular economy and PARC.

Target audience: authorities, international organisations, NGOs, PFAS appliers, PFAS suppliers, remediation companies, research institutes.

Added value: To date, it is still a challenge to detect PFAS in the environment and other media, with estimates of up to ten thousand compounds. It is also not known how many of these substances are relevant to the market and the environment. Analytical chemists are working to develop new methods to fill these gaps.

The EU Partnership for Chemical Risk Assessment (PARC) aims to support chemical management with new approaches to environmental monitoring. The NORMAN network is an important cornerstone of PARC. We want to discuss together which analytical methods are already fit for environmental monitoring, where the challenges lie in assessing the current status of contamination and monitoring the effectiveness of PFAS restriction measures and how in Europe we can join forces for a PFAS-free environment.

PFAS ILS: trifluoroacetic acid & selected PFAS in DW

Interlaboratory studies on trifluoroacetic acid and selected perfluorinated carboxylic and sulfonic acids in drinking water (Leader: IWW, Gerhard Schertzinger g.schertzinger@iww-online.de)

Interlaboratory studies on trifluoroacetic acid and selected perfluorinated carboxylic and sulfonic acids

As an in-kind contribution, together with AQS BW, IWW Water Centre will organise interlaboratory studies on these compounds in drinking or surface water.

- The ILS on trifluoroacetic acid (TFA) will be carried out during the 2nd quarter of 2022
- The ILS on selected perfluorinated acids is scheduled for autumn 2022. Parameters will be: PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFBS, PFPeS, PFHxS, PFHpS, PFOS, PFNS, PFDS, PFUnDS, PFDoDS, PFTrDS. IWW Water Centre, together with AQS BW, will organise interlaboratory studies on the above-mentioned compounds in drinking water.

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

Dissemination of information about the ILS (announcement/invitation, registration form etc) through the NORMAN website and other dissemination channels.

For more technical details and the dispatch dates www.iswa.uni-stuttgart.de/ch/aqs/index.en.html

The proposed budget for this JPA may be revised by the Steering Committee in May 2022. All approved scientific activities will be implemented, independently of the revision of the budget.