

## NORMAN Joint Programme of Activities (JPA 2019)

## List of scientific activities organised by the NORMAN network in 2019

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, taking into account 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.

The Steering Committee has approved a budget of € 276,945 for 2019, based on the expected income from membership fees of the Founding and Ordinary members. These resources will be allocated for scientific and coordination activities (including the NORMAN website), and regular updating and maintenance of the databases.

NOTE: The NORMAN network JPA 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 emerging substances.

Exceptional income of  $\in$  70,000 will be provided by the ICPDR to the NORMAN Association in 2019 as a contribution in support of the NORMAN participation in the experimental activities of the 4<sup>th</sup> Joint Danube Survey (JDS4) to be started in June 2019.

The list of approved scientific activities for 2019 is as follows.

## NORMAN Database System (EI, slobodnik@ei.sk, ipolyi@ei.sk) NORMAN Database Major activities in 2018 were related to the transfer of all, previously scattered, NORMAN database System modules into a common new server and development of the integrated NORMAN Database System (NDS; https://www.norman-network.com/nds/). The NDS consists of 11 modules of which 10 (Suspect List Exchange - SusDat; Chemical Occurrence Data (EMPODAT); Ecotoxicology; Bioassays Monitoring Data; NORMAN MassBank; Digital Sample Freezing Platform (DSFP); Indoor Environment; Passive Sampling; Substance Factsheets; Prioritisation) are already accessible, interlinked and populated with data. The Indoor Environment module is currently using only a small test dataset - more datasets will be provided by WG-6 experts in 2019; the Passive Sampling module will be updated and reprogrammed, following the instructions of CWGA-PS. Antibiotic Resistance Bacteria/Genes is still under development, using the database structure developed within the H2020 Marie Curie ANSWER project. Datasets generated within the project will be uploaded in 2019. All databases can be searched either individually or starting from the module 'Search All Databases'. where the presence of any substance from SusDat in any of the database modules is shown with all existing data. New datasets were uploaded in 2018 into EMPODAT (Chemical Occurrence Data) Database, Ecotoxicology Database and DSFP, using in the background a new extended list of NORMAN substances (SusDat, more than 40,000 substances). Information on curated SusDat substances was completed by data on Lowest PNECs predicted by QSAR (link to Ecotoxicology Database) and mass spectrometric information (exact masses of adduct ions; predicted/experimental fragments) allowing for their search in DSFP. NORMAN MassBank was used to extract experimental fragments, which are essential for identification of suspect substances in DSFP. The design of the Substance

**Scientific activities** 

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Factsheets was improved so as to allow for continuous update with new data on physico-chemical parameters needed for prioritisation and, additionally, Product and Use Categories and Chemical Functional Use information from the US EPA Chemical Dashboard were added. Results from prioritisation case studies performed within the SOLUTIONS project, using the current NORMAN Prioritisation Framework, are available in the Prioritisation module. It is considered important to pursue this effort in collecting data on chemical use categories, classification & labelling (PBT, CMR, ED), Lowest PNECs, hazard properties, exposure indices, etc.
In 2019 upgrade and maintenance of the NORMAN Database System will be pursued with a specific focus on:
<ul> <li>General:         <ul> <li>Interlinking all NDS modules, in particular as regards integration of DSFP, Retention Time Index and Substance Curation tools into the NORMAN Database System;</li> <li>Enhancement of visualisation (maps) and data analysis capabilities (customised queries, batch mode queries using e.g. chemical use categories, chemical functional use information etc.) of NDS.</li> </ul> </li> </ul>
<ul> <li>EMPODAT - Chemical Occurrence Data module:         <ul> <li>Maintenance, upgrading and feeding of new data into the database;</li> <li>Sharing the data with IPCHEM by downloading and sharing the latest update of the EMPODAT Database (annual basis);</li> <li>Further development of a dynamic link between IPCHEM and EMPODAT;</li> </ul> </li> </ul>
<ul> <li>Preparation of JDS4 data for upload into the database;</li> <li>Testing of data mining tools to extract raw data from IPCHEM and other database systems and development of a workflow for their processing into the 'NORMAN format';</li> <li>Testing of automated quality control tools for identification/removal/flagging of outliers in the collected datasets in EMPODAT.</li> <li>Passive sampling module:</li> </ul>
<ul> <li>Finalisation of Passive Sampling module based on the recommendations by CWGA-PS and filling it up with test datasets including new data from the JDS4.</li> </ul>
<ul> <li>ARBs/ARGs module:         <ul> <li>Finalisation of ARBs/ARGs module using the database structure developed within the H2020 Marie Curie ANSWER project;</li> <li>Uploading of data generated within the ANSWER project.</li> </ul> </li> </ul>
<ul> <li>Oploading of data generated within the ANSWER project.</li> <li>Ecotoxicology module:         <ul> <li>Population of the database with new datasets;</li> <li>Further upgrade of the functionalities of the database (e.g. Statistics and Export functions).</li> </ul> </li> </ul>
<ul> <li>SusDat:         <ul> <li>Continuous upgrade and maintenance of SusDat (<i>c</i>. 80,000 new substances in the pipeline);</li> <li>Continuous upgrade of all Data Collection Templates (DCT) for an extended list of NORMAN substances (SusDat), drop-down lists and definitions of obligatory parameters.</li> </ul> </li> </ul>
<ul> <li>Substance Factsheets:</li> <li>Upgrade of Substance Factsheets module – pursue collection of all data needed for the implementation of the NORMAN prioritisation framework.</li> </ul>
<ul> <li>Prioritisation module:         <ul> <li>Implementation/ programming of automated 'Prioritisation module' based on the newly developed prioritisation scheme by WG-1 combining information available on target and non-target screening (semi-quantified) substances (to be discussed/approved at the WG1 meeting in spring 2019 - see Prioritisation WG-1);</li> <li>Update of the Prioritisation results module – visualisation of the results from prioritisation</li> </ul> </li> </ul>
case studies (e.g. SOLUTIONS project) applying the NORMAN prioritisation scheme as a reference.
<ul> <li>Digital Sample Freezing Platform (DSFP):</li> <li>Continuous maintenance and upgrading of DSFP;</li> <li>Upload of new data, including those from the JDS4;</li> <li>Further development and testing of the semi-quantification module;</li> <li>Development and testing of the GC-HR-MS (EI and APCI) modules with new datasets from the JDS4.</li> </ul>
- Implementation of GDPR requirements in NDS.



NORMAN MassBank	NORMAN MassBank and <i>RMassBank</i> (UFZ tobias.schulze@ufz.de and LCSB - Luxembourg emma.schymanski@uni.lu)
and RMassBank	The NORMAN MassBank / RMassBank is part of the NDS and fully interlinked with the other modules, under the supervision of UFZ and LCSB and in consultation of IPB Halle (Germany).
	<ul> <li>In 2019 the continuous development and upgrade of NORMAN MassBank and RMassBank will be pursued with a focus on:</li> <li>Upload of mass spectra to MassBank (UFZ, Eawag, - all NORMAN members welcome!);</li> <li>Further development and curation of RMassBank;</li> <li>Further development of MassBank server platform (e.g. database and applications programming interface, curation of records, import and export of records, standardisation of curation rules);</li> <li>Fostering the integration of MassBank with other mass spectral and metadata platforms (e.g. MoNA, ChemSpider, StoffIdent, US EPA CompTox, NORMAN SusDat);</li> <li>Fostering the discussion with vendors for better integration of vendors' software with MassBank;</li> <li>Improve the usability of MassBank in vendors' software (e.g. via NIST libraries).</li> </ul>
WG-1 Prioritisation of emerging	Working Group N°1: Prioritisation of emerging substances (Activity coordinated by INERIS <u>valeria.dulio@ineris.fr</u> in collaboration with EI <u>slobodnik@ei.sk</u> and UBA <u>peter.vonderohe@uba.de</u> ).
substances	<ul> <li>WG-1 Prioritisation - the following tasks are planned for 2019:</li> <li>Support the prioritisation work of DG ENV / JRC (WFD) at EU level (permanent task): NORMAN will provide a list of candidate substances in 2019 as a contribution to the next update of the EU Watch List planned for 2020;</li> <li>Pursue collection and compilation of ecotox raw data and existing PNECs in support of prioritisation of the substances in SusDat;</li> <li>Ecotoxicology Database: The functionality and the experimental and predicted ecotoxicity data entered in the Ecotoxicology Database already allow for its use in support of prioritisation of ca. 40,000 substances. The focus of WG-1 in 2019 will be on promoting and coordinating participation of Ecotox Expert Group to approve Lowest PNEC values for substances on the SusDat list;</li> <li>Improve the NORMAN prioritisation scheme and testing: a) Finalise the review of the prioritisation study started in 2018 on DSFP data and apply the outcomes in the new NORMAN Prioritisation of CECs in wastewater (see AW-2 "Prioritisation of CECs in urban wastewater");</li> <li>Integrate PMT/vPvM criteria in the prioritisation framework: a) the new parameter for mobility (M and vM) will be integrated in the prioritisation algorithm; b) we will identify PMT/vPvM substances in SusDat based on the proposal by UBA and we will perform a preliminary overview of the target monitoring data available at EU level</li> </ul>
WG-2 Bioassays	Working Group N°2: The value of bioassays and biomarkers in water quality monitoring programmes (Activity coordinated by RWTH – Aachen University <u>Henner.Hollert@bio5.rwth-aachen.de</u> ).
	Task 1: Proof-of-concept application of a biotest battery on samples obtained with large- volume active sampling from the Joint Danube Survey 4 (JDS4) – follow-up of the biotest battery validation study and EBM activities for the WG Chemicals (Leader RWTH, Aachen <u>Henner.Hollert@bio5.rwth-aachen.de</u> )
	This activity is part of the Joint Danube Survey – full project (see detailed description below). In the SOLUTIONS project and within the NORMAN network an integrated set of novel holistic and solutions-oriented monitoring tools has been established to characterise the likelihood of harm



caused by the complex mixtures of chemicals (Brack et al. 2018) <sup>1</sup> . These tools, including effect- based methods (EBMs) and chemical screening techniques, will be exploited in concert with biological and ecological assessments, including DNA-based approaches for a careful assessment within JDS4.
In this JPA the biotests battery recommended by SOLUTIONS and NORMAN (Brack et al., 2019) <sup>2</sup> will be applied on Large Volume Solid Phase Extraction (LVSPE) samples in collaboration with other reference institutes (RWTH, UFZ, RECETOX, INERIS, and others). The monitoring will include <i>in vivo</i> and <i>in vitro</i> testing following the recommendations by SOLUTIONS, NORMAN and the WFD CIS Subgroup on Effect-based methods (EBM). The overall goal of Task 1 is to demonstrate the operational applicability of the EBM battery in the current regulatory framework and its correlation with NTS data.
Task 2: NORMAN Genotoxicity ILS: Data exploitation and publication (Leader: KWR Watercycle Research Institute Milou.Dingemans@kwrwater.nl)
To compare the performance of different bioassays for genotoxicity, a NORMAN interlaboratory study on genotoxicity started in 2018 for blind testing of mixtures of water-relevant genotoxic micropollutants in different <i>in vitro</i> bioassays for genotoxicity and related mechanisms. More than 20 NORMAN members and other organisations participated in this interlaboratory study to test genotoxic activity using many different bioassays. A report on the results of this study was distributed to the participants in February 2019. Additional funding is requested to support the sharing of knowledge and experience of the performance of different assays and data interpretation for genotoxicity assessment and discussion of a peer-reviewed publication on the study (in a workshop, to be confirmed later).
Task 3: Bioassays for the evaluation of neuroactive and neurotoxic emerging pollutants: organisation of a collaborative trial, position paper and workshop (Leader RWTH, Aachen Henner.Hollert@bio5.rwth-aachen.de)
A workshop on Neurotoxicity was organised at RWTH Aachen and a joint paper on neurotoxicity as
an emerging mode of action (MOA) was published based on the workshop (Legradi et al. 2018t) <sup>3</sup> .
Furthermore, a collaborative trial on neuroactive and neurotoxic emerging pollutants was organised by RWTH in 2018 with the following objectives:
<ul> <li>To demonstrate the performance and usefulness of the bioassays on neurotoxicity/behaviour;</li> <li>To write a joint manuscript on the results of the ILS and towards the integration of neurotoxicity as an emerging mode of action (MOA) in a battery of EBMs relevant for water quality monitoring.</li> </ul>
The experiments are finished, the results of the ILS will be submitted to the participants by the end of March 2019 and subsequently a joint manuscript on the results of the ILS will be written (planned autumn 2019).
Task 4: Support the work of the Commission (EBM – CIS WFD Activity) (Leader RWTH, Aachen <u>Henner.Hollert@bio5.rwth-aachen.de</u> )
This activity concerns in particular the proposal for a battery of bioassays for chemical water quality assessment under the WFD and the definition of quality/performance criteria for the benchmarking of

<sup>&</sup>lt;sup>1</sup> Brack W, Escher BI, Müller E, Schmitt-Jansen M, Schulze T, Slobodnik J, Hollert H. Towards a holistic and solution-oriented monitoring of chemical status of European water bodies: how to support the EU strategy for a non-toxic environment? Environmental Sciences Europe 2018; 30: 33.

<sup>&</sup>lt;sup>2</sup> Brack W, Aissa SA, Backhaus T, Dulio V, Escher BI, Faust M, Hilscherova K, Hollender J, Hollert H, Müller C, Munthe J, Posthuma L, Seiler T-B, Slobodnik J, Teodorovic I, Tindall AJ, de Aragão Umbuzeiro G, Zhang X, Altenburger R. Effect-based methods are key. The European Collaborative Project SOLUTIONS recommends integrating effect-based methods for diagnosis and monitoring of water quality. Environmental Sciences Europe 2019; 31: 10.

<sup>&</sup>lt;sup>3</sup> Legradi JB, Di Paolo C, Kraak MHS, van der Geest HG, Schymanski EL, Williams AJ, Dingemans MML, Massei R, Brack W, Cousin X, Begout ML, van der Oost R, Carion A, Suarez-Ulloa V, Silvestre F, Escher BI, Engwall M, Nilén G, Keiter SH, Pollet D, Waldmann P, Kienle C, Werner I, Haigis AC, Knapen D, Vergauwen L, Spehr M, Schulz W, Busch W, Leuthold D, Scholz S, vom Berg CM, Basu N, Murphy CA, Lampert A, Kuckelkorn J, Grummt T, Hollert H. An ecotoxicological view on neurotoxicity assessment. Environmental Sciences Europe 2018; 30: 46.





	bioassays. The aim of this task is to support the implementation of effect-based methods in the regulation as screening tools to reduce the chemical analytical monitoring burden.
WG-3 Effect- directed analysis	Working Group N°3: Effect-directed analysis for hazardous pollutant identification (Activity coordinated by UFZ werner.brack@ufz.de and IVM marja.lamoree@ivm.vu.nl). No new activities of WG-3 will be organised under the NORMAN JPA in 2019. The work of the WG-3 EDA in 2019 will focus on:
	Task 1: Finalisation of the "Virtual EDA" collaborative exercise started in 2017 (see JPA 2017 and 2018) (Leader UFZ, tobias.schulze@ufz.de)
	Mass balances, also known as iceberg modelling, will be used to link effects to chemical results from wide-scope target screening (UFZ). Multivariate statistics will be used to identify chemical signals or targets that correlate with effects if the variance in effects and chemical contamination is sufficiently high to do so.
	The work of the WG-3 EDA in 2019 will pursue the "Virtual EDA" collaborative exercise started in 2017. The aim of this study is to test the virtual EDA concept, where non-target screening data and effect-based measurements are integrated via the application of multivariate analysis, in order to find correlations between effects and typical contamination patterns.
	More than 60 urban WWTPs with different types of treatment have been selected all over Europe. Effluents are collected using a simplified (50 L) LVSPE equipped by UFZ.
	Chemical target- and non-target screening with LC-HRMS and bioanalytical screening with a battery of selected small-volume, high-throughput tests are performed on each sample. The toxicological assessment includes several lethal and sub-lethal endpoints in fish embryo, daphnia and algae as well as a suite of <i>in vitro</i> assays involving endocrine disruption, adaptive stress response, mutagenicity, etc. The sampling campaign, started in 2017, and will be finalised by mid-2019. The analysis will be finalised in 2019. The results are planned to be published in 2020 and ready for upload in NORMAN databases.
	Outcomes: 1) Input to the European discussion on WWTP upgrading; 2) Input to European discussion on effect-based monitoring tools; 3) Input to European discussion on priority pollutants and priority mixtures. The results will be used for joint scientific publication(s) involving all participants and more policy-oriented formats. (Leader: UFZ werner.brack@ufz.de).
WG-4 Engineered	Working Group N°4: Nano- and micro-scale particulate contaminants (Activity coordinated by Eawag – Ralf.Kaegi@eawag.ch and NIVA Bert.vanBavel@niva.no
nanoparticles and	Task 1: ILS on Extraction of engineered nanomaterials from complex matrices (Leader: UFZ, stephan.wagner@ufz.de)
microplastics	ENP released from consumer products and transferred to different environmental compartments cannot yet be detected reliably. An ILS was organised in 2018 to evaluate the performance of specifically-developed sample preparation protocols to extract Au nanoparticles from complex matrices (road runoff, soil and sewage sludge). In September 2018 a workshop on sample preparation protocols was conducted. In total eleven laboratories participated in this activity. The practical laboratory work of this round-robin experiment will be finalised in January 2019, followed by data analysis. A second workshop is planned for 2019, where practical experience from the sample preparation will be shared and the acquired data will be discussed among the participants. The aim of this second workshop is to identify possible pitfalls in the sample preparation procedure and to discuss the data evaluation. Work on the preparation and outline of a manuscript for peer-reviewed publication will also be taken forward during the second workshop.
	Task 2: Microplastics (Leader: QUASIMEME <u>www.quasimeme.org; wim.cofino@wur.nl</u> and NIVA <u>Bert.vanBavel@niva.no</u> )
	An ILS on microplastics will be organised by QUASIMEME in 2019 in collaboration with NORMAN. This study is planned to take place in the first half of 2019, with a follow-up workshop in the second part of 2019 (or early 2020). Information about this study will be distributed through the NORMAN network.
	No funding is requested from NORMAN for this task.
WG-5 Wastewater reuse and	Working Group N°5: Wastewater reuse and contaminants of emerging concern (Activity coordinated by NIREAS, University of Cyprus – Despo Kassinos <u>dfatta@ucy.ac.cy</u> in collaboration with University of Dresden <u>thomas.berendonk@tu-dresden.de</u> ).





contaminants	No new activities of WG-5 will be organised under the NORMAN JPA in 2019.
of emerging concern	Thanks to the ongoing NORMAN collaboration with the EU-funded MSCA ITN project ANSWER, in 2019 it will be possible to proceed to:
	<ul> <li>Finalisation of ARBs/ARGs module using the database structure developed within the ANSWER project;</li> </ul>
	<ul> <li>Uploading of ARBs/ARGs data generated within the project.</li> </ul>
WG-6 Emerging contaminants	Working Group N°6: Emerging contaminants in the indoor environment (Activity coordinated by NILU <u>Pernilla.Bohlin.Nizzetto@nilu.no</u> in collaboration with IVM <u>pim.leonards@ivm.vu.nl</u> and University of Antwerp <u>adrian.covaci@uantwerpen.be</u> ).
in the indoor environment	WG-6 Indoor Environment aims to identify chemicals and chemical groups of emerging concern (CECs) for the indoor environment and to improve the link between indoor emission of CECs and outdoor matrices (waste water, fresh water, surface water, biota etc).
	The work of WG-6 Indoor Environment in 2019 will focus on the following actions:
	<ul> <li>Continue testing of the indoor DCT (including data from passive sampling) by collection and uploading of indoor data in the NORMAN Indoor Environment Database.</li> <li>Improve the master list of substances for prioritisation of CECs relevant for indoor environments by adding use categories, use volumes, and other potentially relevant info for prioritisation process of CECs for the indoor environment.</li> <li>Initiate a follow-up collaborative trial to the previous "Non-target and suspect screening methods"</li> </ul>
	<ul> <li>for organic substances in indoor dust". This CT will focus on European house dust in order to get CECs relevant for Europe and will use harmonised workflows as well as in-house workflows in order to improve the overlap between labs (see ILS-NTS_Dust2).</li> <li>Perform the comparison study of dust sampling methods for CECs (already part of JPA 2018).</li> </ul>
	Two meetings are planned to take place in 2019: a skype-conference and a WG meeting, October 2019 in Umea, Sweden.
Non-target screening Cross- Working Group Activity (CWG-NTS)	CWG-NTS: Cross-Working Group Activity on Non-target screening (Activity coordinated by Eawag juliane.hollender@eawag.ch in collaboration with El slobodnik@ei.sk, University of Athens Nikolaos Thomaidis, <a href="https://nthoa.gr">ntho@chem.uoa.gr</a> , LCSB - Luxembourg <a href="https://www.emma.schymanski@uni.lu">emma.schymanski@uni.lu</a> UFZ <a href="https://www.emma.schymanski@uni.lu">tobias.schulze@ufz.de and NIVA kevin.thomas@niva.no</a> ). The following actions will be carried out as part of the CWG-NTS Activity in 2019:
	<ul> <li>NORMAN Suspect Lists Exchange and associated "SusDat" database: Database development and maintenance (EI, UoA and LCSB,) (see "Suspect List Exchange and SusDat");</li> <li>Second round of the NORMAN network Early Warning System initiative (NormaNEWS2) (NIVA, UoA) (see "NormaNEWS2");</li> <li>NORMAN MassBank - Continuous development and upgrade (UFZ, LCSB and IPB Halle) (see "NORMAN MassBank");</li> <li>Digital Sample Freezing Platform (EI) (see "Databases – NORMAN DSFP");</li> <li>NORMAN Non-target screening guidance paper (UFZ) (see "NTS Guidance document");</li> <li>Development of a semi-quantification method based on advanced chemometrics (UoA) (see "NTS semi-quantification");</li> <li>Proof-of-concept to obtain MassBank records for GC-HRMS data (UoA) (see MassBank GC- HRMS data);</li> </ul>
	<ul> <li>ILS on Impact of deconvolution and library search algorithms for non-target analysis based on a passive sampling approach for non-target analysis screening of polar substances (NIVA) (see ILS NTS data treatment);</li> </ul>
	<ul> <li>ILS on suspect screening in biota: application of a wide-scope suspect screening to compare sample preparation techniques for suspect screening workflows (SLU) (see ILS NTS biota);</li> <li>ILS on non-target screening and suspect screening methods for organic substances in European</li> </ul>
	<ul> <li>indoor dust (Umea University) (see ILS-NTS Dust_2)</li> <li>NTS of CECs in polar regions (EI and UBA) (see "CECs in polar regions")</li> <li>SWEMSA19 workshop on 21-23 October 2019, Erding, Munich, Germany (TUM) (see AW-5)</li> </ul>
	<ul> <li>Investigate the aspects associated with the presence of CECs in aquatic plants (non-target and target screening of plant tissues (full plants such as Lemna sp., etc. and/or plant organs such as P. Australis) with focus on sample and extracts preparation, as an additional topic to be considered within the scope of CWG-NTS (links with on-going research activities on the use of surface-flow wetlands for treated wastewater and stormwater) (University of Lorraine).</li> </ul>

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Passive sampling	CWG-PS - Passive sampling Cross-Working Group Activity (Leader NIVA <u>lan.Allan@niva.no</u> and IRSTEA <u>cecile.miege@irstea.fr</u> ).
Cross- Working Group Activity (CWG-PS)	The work of the Passive Sampling Cross-Working group activity in 2019 will focus on the following tasks:
	Task 1: Analytical and bioanalytical assessments of organic micropollutants in the Danube River using a combination of passive sampling, bioassays and non-target screening: Demonstrating the NORMAN methodology for monitoring purposes in Joint Danube Survey JDS4 (Leader: RECETOX <u>vrana@recetox.muni.cz</u> ) (see Proof-of-concept passive sampling JDS4)
	Task 2: ILS on Impact of deconvolution and library search algorithms for non-target analysis based on a passive sampling approach for non-target screening of polar substances (Leader: NIVA, saer.samanipour@niva.no_and ian.allan@niva.no) (see ILS – NTS data treatment)
	Task 3: Finalisation of the NORMAN Passive Sampling Database (see NORMAN Database System)
CWG-NTS: NORMAN Suspect List Exchange and SusDat	<b>NORMAN Suspect List Exchange</b> (Leader: LCSB, Luxembourg <u>emma.schymanski@uni.lu</u> ) and SusDat (Leader: El <u>slobodnik@ei.sk</u> and Nikiforos Alygizakis <u>alygizakis@ei.sk</u> in collaboration with UoA Nikolaos Thomaidis <u>ntho@chem.uoa.gr</u> and Reza Aalizadeh <u>raalizadeh@chem.uoa.gr</u> ) (Activities organised as part of the CWG Activity on NTS)
	Suspect List Exchange (Leader: LCSB, Luxembourg emma.schymanski@uni.lu)
	The Suspect List Exchange initiative started in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. Connected to the Suspect List Exchange initiative, the compiled Suspect List "SusDat" is today the cornerstone/data basis for all NORMAN databases and prioritisation efforts in NORMAN. For 2019, this Suspect List Exchange activity involves the addition of new lists to the Suspect List Exchange, which can then feed into SusDat. This activity will keep the Suspect List Exchange running at the current state with no additional resources requested at this stage, so that efforts can be concentrated on developing a sustainable SusDat. In 2019 the following actions will be addressed:
	<ul> <li>Addition of new lists when they become available;</li> <li>Website maintenance and development;</li> <li>Integration of DTXSIDs (CompTox identifiers) into lists;</li> <li>Progressive registration of prioritised compounds in lists not present in the CompTox Dashboard;</li> <li>Development of new strategies to deal with UVCBs;</li> <li>Further development of strategies to deal with tentative/unknown/related structures;</li> <li>Publication(s) on methods and software behind Suspect Lists Exchange.</li> </ul>
	Suspect List Exchange Database - SusDat (Leader: El slobodnik@ei.sk and alygizakis@ei.sk)
	In 2018 the Suspect List Exchange (https://www.norman-network.com/nds/susdat/) was integrated into a robust and sustainable database - SusDat (https://www.norman-network.com/nds/susdat/) which today contains more than 40,000 substances compiled from 22 suspect lists, is now fully integrated in the NORMAN Database System (https://www.norman-network.com/nds/). The primary function of SusDat is to provide unique identifiers for substances and their transformation products throughout the various NDS modules and provide information for suspect screening in HR-MS chromatograms uploaded into the NORMAN Digital Sample Freezing Platform (DSFP). Assigning correct names, CAS No., InChIKeys, SMILES etc. was performed in close cooperation with the US EPA CompTox Dashboard team (https://comptox.epa.gov/dashboard). In order to facilitate use of SusDat in DSFP, a Retention Time Index (RTI) was assigned to all substances by UoA, and mass spectrometric information (exact mass of adduct ions and fragments) was added by EI. Experimentally-obtained fragments by NORMAN MassBank (http://massbank.eu/MassBank/) were used as the primary information.
	Lists Exchange and SusDat in a way that will support all the NORMAN efforts. In particular the following tasks are planned for 2019:
	<ul> <li>Suspect List Exchange website maintenance and update;</li> <li>Addition of new lists in Suspect List Exchange website when they become available;</li> </ul>



	<ul> <li>Update of SusDat with combined list of all suspects with MS-ready forms from individual lists;</li> <li>Further development of SusDat functionalities (e.g. batch mode queries based on chemical use categories, chemical functional use etc.);</li> <li>Testing of auto-curation tool developed by UoA and ability for users to add their own lists;</li> <li>Publication(s) on methods and software behind Suspect List Exchange and SusDat.</li> </ul>
CWG-NTS: NormaNEWS and retrospective screening	NormaNEWS and retrospective screening (Leader: NIVA kevin.thomas@niva.no; saer.samanipour@niva.no_in collaboration with EI Nikiforos Alygizakis alygizakis@ei.sk and UoA, Nikolaos Thomaidis ntho@chem.uoa.gr) (Activity organised as part of the CWG Activity on NTS) The concept of NormaNEWS is that when one group identifies a new contaminant of emerging concern, identification criteria are sent to other members of the group who use retrospective analysis techniques to check their own samples. This way it is possible to rapidly establish the occurrence of newly identified compounds of emerging concern across Europe and beyond (thereby contributing to identification of future priority contaminants). The first round of the collaborative NormaNEWS joint activity in 2016 successfully demonstrated the usefulness of the retrospective screening of high-resolution mass spectrometric (HRMS) data in establishing the spatial and temporal occurrence of newly identified compounds of emerging concern. To build on the first study, a second NormaNEWS exercise will be performed in 2019 (postponed, initially planned to take place in 2018). The objective is to further develop the approach and cover many more contaminants of emerging concern in NormaNEWS2, including a broader range of matrices, and significantly increase temporal and spatial coverage. Expression of interest to participate is currently open and submission of novel suspects through the following portal ( <u>http://normanews.eu/</u> ) will be possible until 1.5.2019.
CWG-NTS: NTS Guidance document	NORMAN Non-target screening guidance paper (Leader: UFZ, martin.krauss@ufz.de) Non-target screening (NTS) using LC-HRMS for the monitoring of aquatic environments within the research community has seen rapid development over the last decade. A considerable number of different analytical and instrumental approaches and data processing workflows have been developed. Its high potential has raised the interest of authorities at different levels in applying NTS in monitoring, prioritisation of compounds and assessment of treatment technologies within regulatory frameworks. To address this interest NORMAN organised a workshop in 2018 specifically addressed to stakeholders: "Non-target screening for regulators: How can non-target screening techniques support environmental monitoring and chemicals management?". Various regulatory bodies repeatedly expressed the need for guidance on a "best practice" document for setting up and running NTS, and harmonisation of approaches as a condition to apply them on a routine basis within their respective frameworks. The overall goal of this action is to provide a guidance document on NTS with a focus on the needs of regulators and policy-makers. The final document should be ready by early 2020, with the aim of a publication in an open access and peer-reviewed journal.
CWG-NTS: NTS semi- quantification	<b>Development of semi-quantification method based on advanced chemometrics</b> (Leader: University of Athens, Nikolaos Thomaidis





The work will consist of the following tasks:
Task 1: Chemometric tools and analyses will first be used to identify a set of compounds as an internal calibration set for semi-quantification purposes. These compounds will be representative of chemical properties, elution pattern in liquid chromatographic systems and instrumental response factor (ionisation efficiency and concentration ranges).
Task 2: These calibrants will be internally tested on artificial suspects at various concentration ranges. The outcomes will be discussed within NTS CWG in order to agree on subsequent actions such as external evaluation, improvement of workflows, etc.
Task 3: The proposed semi-quantification method will be externally evaluated at UFZ, EI, EAWAG, INERIS, NIVA and NILU to provide proof-of-concept and to measure its accuracy across different LC and MS instrumentation.
Task 4: Development of an open-source software to perform semi-quantification over suspect compounds.
The following outcomes are expected by the end 2020:
<ul> <li>A framework to estimate concentrations of suspects by a novel semi-quantification approach in RPLC-HRMS;</li> </ul>
<ul> <li>Evaluation of the semi-quantification strategy in various RPLC-HRMS systems;</li> <li>Development of an open-source software to perform semi-quantification over suspect compounds;</li> </ul>
<ul> <li>Publication(s) on the methods and software behind this semi-quantification approach.</li> </ul>
Proof-of-concept to obtain MassBank records for GC-HRMS data (Leader: University of Athens, Nikolaos Thomaidis <u>ntho@chem.uoa.gr</u> )
In the emerging contaminants (ECs) analysis field, there is a clear trend toward LC-HRMS, as the majority of new ECs are more polar, less volatile and thermostable and, consequently, less GC-amenable. However, still a significant number of the high-usage ECs and priority pollutants are volatile and thermostable. Therefore, GC-HRMS methods should be developed to extend the chemical domain of the applied screening approaches.
The development of HRMS spectral databases, such as MassBank, has been proven to be a vital tool to support the identification of suspects and unknowns as well as to reduce false positive findings. The need to enrich MassBank with GC-HRMS records obtained by different sources and mass spectrometers (e.g. GC-APCI-QTOFMS, GC-EI-QTOFMS and GC-EI-Orbitrap) becomes evident.
This activity will contain two main/separate parts, which are: (1) evaluation of the RMassBank workflow for the processing of GC-HRMS mass spectra and (2) the analysis of a test set of environmentally relevant GC-amenable reference standards in different state-of-the-art GC-HRMS instruments by the core members of this JPA (UoA: GC-APCI-QTOFMS; UFZ: GC-EI-Orbitrap and WRI: GC-EI-QTOFMS). The objective is to obtain a better understanding of the differences between the three acquisition techniques, and to establish knowledge, background and a strategy for the creation of high-quality GC-HRMS data for future MassBank records.
Analytical and bioanalytical assessments of organic micropollutants in the Danube River using a combination of passive sampling, bioassays and non-target screening: Demonstrating the NORMAN methodology for monitoring purposes in Joint Danube Survey JDS4 (Leader: RECETOX, <u>vrana@recetox.muni.cz</u> )
This activity is part of the Joint Danube Survey – full project (see detailed description below).
Passive samplers can accumulate pollutants, just as organisms do, and concentrate sufficient amounts of pollutants from water for chemical and toxicological analysis where spot sampling methods often fail. NORMAN has already successfully demonstrated applicability of PS for chemical and effect-based monitoring of a broad range of organic chemicals in the previous JDS3 survey (Novák et al. <sup>4</sup> , 2018; Vrana et al., 2018 <sup>5</sup> ).

<sup>&</sup>lt;sup>4</sup> Novák, J., Vrana, B., Rusina, T., Okonski, K., Grabic, R., Neale, P.A., Escher, B., Macova, M., Ait-Aissa, S., Creusot, N., Allan, I., Hischerova, K., 2018. Effect-based monitoring of the Danube River using mobile passive sampling. Sci. Total Environ. accepted. <sup>5</sup> Vrana, B., Smedes, F., Allan, I., Rusina, T., Okonski, K., Hilscherová, K., Novák, J., Tarábek, P., Slobodník, J., 2018. Mobile dynamic passive sampling of trace organic compounds: Evaluation of sampler performance in the Danube River. Sci. Total 9

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	The proposed application of a temporally-integrative sampling approach will result in samples that provide a representative picture of the pollution situation at 10 defined sites on the Danube river. Passive samples from water will be investigated by target chemical analyses (priority and river basin specific pollutants), non-target screening and toxicity profiling by a battery of NORMAN/SOLUTIONS bioassays used also for analyses of JDS4 LVSPE samples.
	Objectives:
	<ul> <li>Provision of a methodology and setting-up a baseline for representative monitoring of trace organic pollutants in large water bodies, enabling the setting-up of long-term trend monitoring of relevant substances;</li> <li>Identification of toxicity drivers in complex pollutant mixtures present in the Danube river;</li> <li>Identification of bioaccumulative substances based on comparison of chemical mixtures present in passive sampler extracts from water and biota using non-target screening.</li> </ul>
Joint Danube Survey – full	Collaborative activities NORMAN – ICPDR Joint Danube Survey 4 (JDS4) (Leader: EI in coordination with UFZ)
project	The Danube surveys have been organised every six years since 2001 under the leadership 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 approved by Water Directors of all involved countries and DG Environment. JDS4 is planned to start on 29 June 2019.
	The key objective of JDS4 is to produce comparable and reliable information on selected water quality elements for the whole length of the Danube River, including the major tributaries on a short-term basis and to provide an opportunity for harmonisation and training in WFD-related monitoring.
	A JDS4 brainstorming workshop involving experts from the ICPDR and NORMAN network took place in Bratislava on 6-7 Sept 2018. Areas of common interest between NORMAN and JDS4 were identified and translated into several NORMAN JPA 2019 proposals (see details in the Factsheet), including activities such as analysis of a wide-scope and wide polarity range of emerging substances at trace levels, non-target screening (NTS) and effect-based monitoring (EBM), which are addressed in depth by the NORMAN network. JDS4 offers NORMAN experts an excellent 'playground' for testing different analytical and monitoring tools on a large transboundary river basin. The overall goal is to demonstrate the practicality of use of the new analytical techniques (EBM, NTS, passive sampling, etc.) in the current regulatory framework.
	The following activities will be carried out in 2019: Samples will be taken by the JDS4 National Teams at 51 sites and a full-scale biological (WFD Biological Quality Elements; zooplankton etc.), chemical (WFD priority substances, provisional Danube River Basin Specific Pollutants (RBSPs), substances in the 'Compound Fishing' list of JRC Ispra etc.), radiological and hydromorphological assessment will be carried out. Analyses of microplastics (UBA Germany) will be performed in samples from 9 sites. NORMAN partners will analyse either all samples from the 51 sites or focus on 20-25 'supersites' where more in-depth investigations will be carried out. Samples from these sites will undergo, <i>i.a.</i> , a thorough eDNA screening, microbiology, and antibiotic resistance genes/bacteria (ARGs/ARBs) analyses. Additionally, samples from
	<ul> <li>10 WWTPs (effluent; 7-days composite or large volume SPE)</li> <li>10 ground water sites (bank filtration)</li> <li>10 biota samples</li> </ul>
	• 10 passive samplers will be included. Altogether 91 sets of samples of water, sediment, SPM, biota and passive samplers' extracts will be available. Samples for the above analyses will be collected by a group of experts travelling alongside the Danube by cars. Passive sampling, sampling of waste water effluents and ground water will be organised independently.
	The distribution of samples and analyses is as follows: 1. Large volume SPE (LVSPE) water and SPM samples will be collected by MAXX sampler (UFZ) for (i) wide-scope target analysis (>1200 substances) and upload of raw data into

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	the NORMAN Digital Sample Freezing Platform (DSFP) for <b>retrospective suspect</b> <b>screening</b> of water samples by LC-HR-MS and GC-HR-EI-MS; (ii) specific target screening for <b>steroids and aromatic amines</b> ; (iii) analysis by a NORMAN/SOLUTIONS battery of high-throughput <i>in vitro</i> <b>bioassays</b> incl. ARE, Erα, AR, GR, PPARγ, AhR (UFZ), µEROD, Ames Fluc, µNucleous (RWTH) and (iv) <b>small-scale apical tests</b> with miniaturized algae, Daphnia and FET assays (UFZ); (v) additional <b>wide-scope target screening of SPM</b> <b>samples</b> by LC-HR-MS (UFZ).
•	Samples: 30 L; 50 L at three selected intercomparison sites; collected at the 51 JDS4 sites. Possibility to share aliquots of sample extracts with other interested NORMAN partners.
2.	<b>LVSPE water samples</b> will be collected by Horizon field sampler (EI) for (i) <b>wide-scope target screening</b> (>2400 substances) by LC-HR-MS and GC-HR-APCI-MS (UoA/EI) with specific focus on <b>antibiotics and their transformation products and illicit drugs</b> ; (ii) upload of raw data into DSFP for <b>retrospective suspect screening</b> (EI/UoA); (iii) LC-HR-QTOF-MS, GC-HR-QTOF-MS and upload of raw data into DSFP for <b>retrospective suspect screening</b> (WRI); (iv) GC-LR-MS(MS) (EI/PCI/NCI) (EI) and (v) genotoxicity (UB). Samples from three intercomparison sites will be collected for analyses by a NORMAN/SOLUTIONS battery of high throughput <i>in vitro</i> <b>bioassays</b> incl. ARE, Erα, AR, GR, PPARγ, AhR, µEROD, Ames Fluc, µNucleous (RWTH, UFZ, RECETOX).
•	Samples: 30 L; 50 L at three selected intercomparison sites; collected at 25 supersites. Possibility to share aliquots of sample extracts with other interested NORMAN partners.
3.	<b>Passive sampling</b> (RECETOX); extracts to be analysed for (i) <b>target substances</b> (RECETOX); (ii) <b>wide-scope target screening</b> by LC-HR-MS and GC-HR-MS (UFZ, UoA); (iii) upload of raw data into DSFP for <b>retrospective suspect screening</b> (UFZ, EI/UoA) and (iv) analysis by a battery of NORMAN/SOLUTIONS <b>bioassays</b> incl. ARE, Era, AR, GR, PPARY, AhR, $\mu$ EROD, Ames Fluc, $\mu$ Nucleous (UFZ, RWTH, RECETOX).
•	Samples: 10 sites to be nominated by/agreed with JDS4 national coordinators; need for secure sites protected from theft of samplers; must be the same sites as for fish sampling. Possibility to share aliquots of sample extracts with other interested NORMAN partners. See also "Proof-of-concept passive sampling JDS4" above.
4.	Sediment samples extracts for wide-scope target and suspect (DSFP) screening by LC- HR-MS and GC-HR-EI-MS (UFZ) and LC-HR-MS and GC-HR-APCI-MS (UoA/EI).
•	Samples: 0.5 L of fine sediment; upper 5 cm layer; 63 um fraction; up to five samples as a sub-selection of 25 supersites; must be the same sites as for eDNA analysis.
5.	Water samples for direct injection LC-HRMS (UFZ); wide-scope target and suspect (DSFP) screening; 20 mL sample; all JDS4 water samples (51 surface water, 10 ground water, 10 WWTPs effluents).
6.	Water samples for direct injection LC-HR-MS (TUM); screening of very polar compounds; 20 mL sample; all JDS4 water samples (51 surface water, 10 ground water, 10 WWTPs effluents). Upload of raw data into DSFP for retrospective suspect screening.
7.	Water samples for on-line SPE LC-HR-MS (LfU); wide-scope target screening with special focus on pesticides and their TPs; 50 mL sample; all JDS4 water samples (51 surface water, 10 ground water samples and 10 WWTPs effluents – without SPE). Upload of raw data into DSFP for retrospective suspect screening.
8.	Water samples for LC-HR-MS (LW Langenau); wide-scope target screening and upload of raw data into DSFP for retrospective suspect screening; analysis of samples by four <b>bioassays</b> after HPTLC fractionation incl. AF, BS, AChE, YES; 2 L sample from 10 ground water and 10 WWTPs effluent samples; aliquot of an extract from the 51 JDS4 water samples provided by UFZ.





	9. Biota (fish) samples for wide-scope target screening by LC-HR-MS and GC-HR-EI-MS (UFZ) and LC-HR-MS and GC-HR-APCI-MS (UoA/EI); analysis and upload of raw data into DSFP for retrospective suspect screening (UFZ, UoA/EI, WRI); 10 pooled samples of 10 specimen of agreed upon species/ length; must be the same sites as for passive sampling and eDNA. Lyophilisation at UoA; sample extracts to be delivered to UFZ and WRI for analysis.
	<ol> <li>Water samples for analysis of Dissolved Organic Matter (DOM) and Rare Earth Elements (REE) (UoL); DOM: 2 to 4 L sample, GF/F; REE: 125 mL sample, 0.45 μm filtered; JDS4 water samples (51 surface water, 10 ground water).</li> </ol>
	11. <b>Proof-of-concept application of a biotest battery on JDS4 samples obtained with</b> <b>LVSPE</b> – follow-up of the biotest battery validation study and EBM activities for the WG Chemicals; biotest battery will be used for an investigation of LVSPE samples (UFZ) by RWTH, UFZ, RECETOX and other interested NORMAN partners. The monitoring shall include <i>in vivo</i> and <i>in vitro</i> testing following the recommendations by SOLUTIONS, NORMAN and the WFD CIS subgroup on bioassays: anti/estrogenicity, dioxin-like activity, anti/androgenicity, GR-mediated activity, mutagenicity, FET, Daphnia assay, algae assay. Mass balances, also known as iceberg modelling, will be used to link effects to chemical results from wide-scope target screening (UFZ). Multivariate statistics will be used to identify chemical signals or targets that correlate with effects if the variance in effects and chemical contamination is sufficiently high to do so. For details, see also WG-2 and WG-3 activities above.
	Each of the above activities is being discussed between EI and responsible partners in order to avoid overlaps and increase synergies. Activities of involved NORMAN partners are also a part of the JDS4 Survey Plan (prepared by the ICPDR). Results of the JDS4 – NORMAN activities will be published in the JDS4 Final Scientific Report in 2020.
	Expected outcomes for 2019:
	All data obtained from analyses of JDS4 samples will be uploaded in the NORMAN Database System; ready for further evaluation in 2020 (Workshop NORMAN – ICPDR 2020).
AW-1	Workshop on Environmental Epigenetics - From Mechanisms to Regulation (Leader: Örebro University, Steffen Keiter <u>Steffen.Keiter@oru.se</u> )
	Exposure to environmental pollutants can cause epigenetic changes that may lead to adverse health outcomes in the same generation, and possibly also in subsequent ones, even if these generations are no longer exposed. Thus, there has been growing concern that epigenetic changes by pollutants may mediate adverse health outcomes over several generations. Epigenetics is mediating long-term regulation of gene expression, which allows different phenotypes without changes in DNA sequence.
	The aim of this workshop is to give an overview of the topic and share within NORMAN detailed current knowledge and results of recent investigations (www.oru.se/epigeneticworkshop/english).
	The workshop is already supported by Örebro University and other organisations, including IFREMER, SWETOX, etc. The additional NORMAN contribution is requested to cover travel expenses for invited guest speakers. Date of the workshop: 21-22 February 2019.
WG-1	Workshop on Prioritisation of contaminants of emerging concern in urban wastewaters
Prioritisation AW-2	(Leader: INERIS, <u>valeria.dulio@ineris.fr</u> ) Several existing EU Directives (Urban Waste Water Treatment Directive, Water Framework Directive,
	etc.) are undergoing an evaluation process (Fitness-check). In support of this policy review process, various EU projects have been funded to tackle the problems/risks of CECs in urban wastewater.
	A one-day workshop will be 12rganize12 under the NORMAN umbrella in collaboration with the EU- funded AQUAlity ETN project (https://www.aquality-etn.eu/) in order to:



	<ul> <li>Provide an overview and critical analysis of the results of the most relevant on-going initiatives and;</li> </ul>
	<ul> <li>Discuss the position of the experts on a possible European "priority" list of CECs in wastewater, the most relevant groups (of compounds) for innovative treatment technologies, revision of emission limit values (LV) and control measures, in the context of the on-going policy review process.</li> </ul>
	The workshop will take place on 6 March 2019 at Ecole Polytechnique, Palaiseau, Paris, France, back-to-back with the Winter School on Mass Spectrometry Analysis 13rganize13 by the Ecole Polytechnique (Palaiseau, France).
WG-1 Prioritisation AW-3	Workshop on Persistent, mobile and toxic (PMT) substances: a challenge for analytical chemistry and water quality control (Leader: UFZ, <u>urs.berger@ufz.de</u> and <u>thorsten.reemtsma@ufz.de</u> in collaboration with KWR, <u>Stefan.Kools@kwrwater.nl</u> and UBA, <u>michael.neumann@uba.de</u> and <u>Peter.VonderOhe@uba.de</u> )
	Persistent and (very polar) mobile substances (PM substances) are a potential threat to water quality. A protection gap exists for drinking water. Only dilution helps to reduce environmental concentrations of PM substances. Moreover, an analytical gap exists because LC-MS screening and monitoring do not cover highly mobile contaminants.
	This 1½ day workshop aims to foster the scientific development necessary to improve our abilities to evaluate the significance of PM (PMT) substances for water quality and drinking water supply. Focus:
	<ul> <li>Highlighting the present state of methods and knowledge of PM substances;</li> <li>Identifying the obstacles and shortcomings in the different fields of research on PM substances;</li> <li>Proposing strategies for overcoming them.</li> </ul>
	The workshop will build on the outcomes of the recent European Water JPI project PROMOTE and will be supported by a new research project on PM compounds (2019–2021) led by UFZ.
AW-4	Expert Group meeting on NTS and eDNA (Leader: EI, slobodnik@ei.sk)
	A large amount of data is generated by NTS and eDNA approaches. The possibility of combining them and searching for a correlation between chemical pollution and biological response was identified as of high interest for many members of the NORMAN network at the 2017 GA in Leipzig. NTS and eDNA (for benthic invertebrates, fish and diatoms) approaches will be tested within the JDS4 in 2019 and unique datasets will become available for further evaluation.
	The aim is to organize a meeting of interested NORMAN network and DNAquaNet COST Action experts; possibly back-to-back with the WG1 meeting in spring 2019 to define a programme for evaluation of results from JDS4 and fine-tuning of the survey programme.
NTS-CWG: AW-5	SWEMSA19 workshop on Non-Target Screening embedded in (Open Access) Platforms and Multi-disciplinary Applications (Leader: TUM, Thomas Letzel in collaboration with Eawag, juliane.hollender@eawag.ch , UFZ, tobias.schulze@ufz.de and martin.krauss@ufz.de , University of Luxembourg, emma.schymanski@uni.lu Environmental institute, slobodnik@ei.sk ; Alygizakis alygizakis@ei.sk ;
	Further to the success of "SWEMSA 16" in Garching, this second edition of the SWEMSA (Solutions and Workflows in (Environmental) Molecular Screening and Analysis) events will bring together international leading scientists from international consortia. SWEMSA informs, combines and intends to harmonise NTS strategies and workflows from each single discipline to extend the NTS horizon and to give to all different communities of users the chance to 'have a look over the edge'. Participants from various disciplines such as, chemistry, food, forensic, informatics, metabolomics and instrumental analysis will jointly discuss latest developments. The programme will feature a solution-focused discussion strategy including panel discussions and overview talks.
	The overall aim of this meeting is to condense and harmonise various common aspects of NTS, to extend the use of software and workflow strategies and give the opportunity to learn about the potential of NTS applied in various disciplines.
	The workshop will take place on 21-23 October in Erding, Munich, Germany.
CECs in polar regions	<b>CECs in polar regions: Collection of samples and their analysis</b> (Leader El <u>slobodnik@ei.sk</u> and UBA jan.koschorreck@uba.de)



NTS of biota samples is becoming an important issue in NORMAN activities. Pollutants preser biota are highly probably bio-accumulative (B) and persistent (P), and thus fulfilling two out of th PBT criteria considered under REACH legislation. Up to now, most of the efforts of research gro worldwide were focused on analysis of target substances in biota. In 2018, NORMAN has suppo LIFE APEX project 'Systematic use of contaminant data from apex predators and their pre- chemicals management', which will run till 2022. A part of the project deals with development target and mathematical for agemptic application, and which are the project deals with development	nree
standardised methodologies for sample collection, preparation and analysis, including wide-sc target, suspect and non-target screening. Aspects of standardisation of biota NTS analysis were discussed at the NTS of biota workshop in Upssala, Sweden in October 2018.	rted y in nt of cope
As a means of prioritising the most ubiquitous pollutants at the global scale there is a need to loo their occurrence in remote areas, including the Arctic region and Antarctica. NORMAN members h access to samples from these regions. It is expected that with the global warming the polar areas become more accessible and, thus, more polluted from anthropogenic activities. A baseline pollution by several target substances has already been developed within the AMAP proj However, we are not aware of studies systematically setting up such a baseline by NTS approach	ave will e of ject.
The following activities will be carried out in 2019:	
<ul> <li>Collection of ca. 20 samples representing various trophic levels (e.g. sea stars, fish, a predators) available in Environmental Specimen Banks or provided by NORMAN partr covering Antarctica and Arctic region and their analysis by a wide-scope target, suspect and r target screening approach developed within the APEX project. Coordination of the develo workflow with the ILS-NTS biota activity (see Factsheet);</li> <li>Testing amenability of LC-HRMS and GC-HRMS methodologies for NTS of matrices not inclu in the APEX project (e.g. blood, eggs, etc.).</li> <li>Organisation of a workshop discussing the obtained results with a possibility of launching lau scale project at the EU level.</li> </ul>	ners non- ped ded
Expected outcomes for 2019:	
All data obtained from analyses of samples from the polar regions uploaded in the NORM Database System (EMPODAT and DSFP).	1AN
Demonstration of the use of DSFP for retrospective screening of selected suspected persistent bio-accumulative substances.	and
NTS-CWG:         ILS on Impact of deconvolution and library search algorithms for non-target analysis ba on a passive sampling approach for non-target screening of polar substances (Leader: NI saer.samanipour@niva.no_and lan.Allan@niva.no) (Activity organised as part of the CWG-NTS the CWG-Passive Sampling)	IVA,
NORMAN has already organised several ILS in order to assess the quality/confidence in identification of small organic molecules in different matrices (e.g. NormaNEWS). However, on the steps that has yet to be evaluated is the deconvolution and library search algorithms. therefore propose an ILS where we evaluate the effect of each step during the data processing the outcome of NTS. This project will also focus on streamlining the use of passive sampling in NTS workflow by demonstrating the advantages to the NTS of using this sampling strategy. activities in this project will therefore be divided into two parts: passive sampling and NTS.	e of We g on the
- Passive sampling:	
- rassive sampling.	river
We will work on a scenario of release of sewage treatment plant effluent in a relatively clean r with passive sampler deployment upstream, downstream and in the effluent itself. The objective sample analysis will be to screen and identify (some of) the polar chemicals originating from effluent and present at the downstream sampling site. Passive samplers will be deployed for exposure durations. We plan to use one type of passive sampler (to be decided). We will confirm emission and presence of 20-50 relevant chemicals in the various extracts through target analysis the organisers. These chemicals will be followed throughout the NTS and suspect screening proc undertaken by participating laboratories.	e of the two the s by
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WG-6 Indoor env:	<b>Collaborative Trial for dust sampling protocols</b> (Leader: IVM Pim Leonards, pim.leonards@ivm.vu.nl in collaboration with University of Antwerp Adrian Covaci
	The finalisation of the study will take place in 2020, including: Data collection and upload in DSFP and NORMAN Indoor Environment Database; Data evaluation; Organisation of a 2 <sup>nd</sup> workshop to discuss results and method evaluation; Preparation of a scientific publication.
Dust_2	<ul> <li>previous CT, ii) propose improved workflows, including the use of SusDat, indoor dust contaminant suspect lists and DSFP, iii) choose a harmonised workflow method for the study (planned for 2019);</li> <li>Dust sampling collection, dust homogenisation and distribution.</li> </ul>
	<ul> <li>The main steps for the organisation of this action planned to take place in 2019 are:</li> <li>Organisation of a preparatory meeting/training workshop to: i) discuss experiences gained in</li> </ul>
	It is proposed to organise a Collaborative trial on non-target and suspect screening methods using the GC-MS and LC-HR-MS(MS) methodologies available in participating laboratories using both harmonised workflows and in-house workflows. The aim of this CT is to have a follow-up action to build on the experience from the previous NORMAN CT: "Non-target and suspect screening methods for organic substances in indoor dust".
NTS-CWG and WG-6 Indoor env: ILS-NTS	ILS on Non-target and suspect screening methods for organic substances in European indoor dust (Leader: Umeå University <u>peter.haglund@chem.umu.se</u> , NILU Pawel Rostkowski; Pernilla Bohlin-Nizzetto; Antwerpen University Adrian Covaci; IVM Pim Leonards; El Nikiforos Alygizakis, Peter Oswald
	<ul> <li>Expected outcomes for 2020:</li> <li>The data evaluation will be carried out by the organising committee;</li> <li>A final workshop including all participants will be organised in the third quarter of 2020 and a scientific publication on the results of the ILS is expected in 2021.</li> </ul>
	The ILS preparation will start in summer 2019 including homogenisation, spiking of samples, and testing of homogeneity of the samples. The whole fish lyophilised homogenates and reporting protocols will be sent out to participants during the third quarter of 2019. Participants will have time to contribute with their results until spring 2020.
	Fish will be sampled in spring 2019 (contaminated vs reference site).
	<ul> <li>Investigate the performance of the sample preparation methods with the aim to reach consensus on a harmonised sample preparation protocol;</li> <li>Compare suspect screening workflows;</li> <li>Reveal the range of chemicals detectable in fish tissue.</li> </ul>
	Of the fortified substances, 10 will be known by the participants in advance for control purposes, while it will be up to the participants to identify the remaining 40 substances. The aim of this study is to:
	<ul> <li>Whole fish homogenates from a contaminated and reference site (e.g. upstream vs downstream);</li> <li>Whole fish homogenates non-spiked and spiked with <i>c</i>. 50 emerging organic micropollutants.</li> </ul>
	Suspect and non-target investigation of biota samples collected by Environmental Specimen Banks (ESBs) is a topic of growing interest. In this collaborative trial researchers from universities, food agencies and research institutes will analyse:
NTS-CWG: ILS-NTS biota	ILS on suspect screening in biota: Application of wide-scope suspect screening to compare sample preparation techniques for suspect screening workflows (Leader: SLU, lutz.ahrens@slu.se, wiebke.durig@slu.se in collaboration with Stockholm University, jon.benskin@aces.su.se, Umeå University peter.haglund@chem.umu.se and El alygizakis@ei.sk)
	participating labs will be asked to generate the Open format raw data, peak lists, and the IDs of the detected and identified features. We will provide the participants with the necessary reporting templates for ease of QA/QC. All the results will finally go through a QA/QC step performed by the organisers in order to evaluate the reasons behind potential misidentifications (e.g. less than two fragments extracted and/or large mass error). Additionally, other QA/QC measures will be used to further assess the reason behind false detections.





ILS-Dust	adrian.covaci@uantwerpen.be and NILU Pernilla.Bohlin.Nizzetto@nilu.no) (Activity organised as
sampling	part of WG-6 "CECs in indoor environment")
	In the last decade, an increasing number of papers have reported the levels of SVOCs (semi-volatile organic compounds) in indoor dust and air. Different sampling protocols and equipment are used to collect indoor dust, but no standardised protocol is available. Different sampling protocols can result in different particle size fractions collected. There is a great need for an intercomparison study on dust sampling protocols to evaluate whether different sampling methods and sample treatments (e.g. sieving) can cause differences in SVOC levels.
	The activity was planned to take place in 2018 (see JPA 2018), but due to logistic problems it has been postponed to 2019.
	The following activities will be carried out in 2019:
	<ul> <li>Set up an intercomparison study of dust sampling and treatment using different sampling protocols (for this study, a commercially available SRM dust material will be used);</li> <li>Determine the levels of specific emerging and legacy SVOCs (e.g. PBDEs, nBFRs, OPFRs, PAHs, Phthalates, PFAS, PCBs and OCPs) in these samples;</li> <li>Reporting of the results (planned in 2019).</li> </ul>
	A scientific paper will be produced.
ILS-IWW	Interlaboratory studies on sweeteners, benzotriazoles, and selected pharmaceuticals (Leader: IWW as full in-kind contribution, David Schwesig <u>d.schwesig@iww-online.de</u> )
	Together with AQS BW, IWW Water Centre will organise interlaboratory studies on these compounds in drinking water, as follows:
	<ul> <li>The ILS on sweeteners and benzotriazoles is scheduled for April 2019 (registration deadline 15 Feb 2019). Parameters will be acesulfame, cyclamate, saccharine, sucralose, 1H-benzotriazole, 4-methyl-1H-benzotriazole, 5-methyl-1H-benzotriazole, Sum of methyl-1H-benzotriazoles);</li> <li>The ILS on selected pharmaceuticals is scheduled for September 2019 (registration deadline 12 July 2019). Parameters not yet defined.</li> </ul>
	The studies will combine proficiency testing of laboratories and evaluation of the suitability of methods used (NORMAN Validation level: V3 - routine).
	Information about the ILS (announcement/invitation, registration form etc.) will be disseminated through the NORMAN website and other dissemination channels.
	No financial contribution needed
	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 2019. All approved scientific activities will be implemented, independently of the revision of the budget.