

Proposals for NORMAN Joint Programme of Activities 2022

Title	NORMAN WG Prioritisation activities
Type of activity	Working Group activities
Leader	INERIS in collaboration with EI and UBA in collaboration with Ecotoxcentre
Topic / activities	<p>Background / Justification for the proposed activity:</p> <p>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 the most urgent actions necessary to achieve these goals.</p> <p>In 2021, the new version of the NORMAN prioritisation framework, combining target and suspect-screening data, has been tested on a large-scale case study. A number of tools – IP score, semi-quantified data approach, EMPODAT-Suspect Database, automated prioritization tool – have especially been 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 (Task 6, 7 and 8), taking in mind 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.</p> <p>The NDS Ecotoxicity Database module has also been improved, with now almost 65,000 substances covered by predicted PNECs and more than 5,000 compounds for which experimental toxicity studies are available. The Ecotoxicity module has also gained in performance thanks to the implementation of new functionalities. However, most of the data are related to the water compartment and it is necessary now to put more effort to extend the scope to new compartments and also to new prioritisation objectives. For example, it should be possible to derive protection values for reuse of reclaimed water in agriculture and prioritise the compounds which need to be controlled in the water resource before use in agriculture (see Task 2 and Task 3).</p> <p>Compilation of information about the physico-chemical characteristics and hazardous properties of the compounds has been improved. For example as regards the evaluation of the PBT and PMT criteria, a P score is now assigned to 65,000 compounds in the SusDat list, thanks to the fruitful cooperation with UBA and the implementation of the JANUS model for prediction of PBT criteria in the NDS.</p> <p>The next step for improvement of the prioritisation activities will be the systematic collection and classification of information about the uses of the compounds and the development of approaches to group the compounds based on their use(s), functional groups, modes of action, etc. (see Task 5).</p> <p>We need also to consider mixture toxicity effects and identify the compounds which – even if they are not exceeding threshold values individually – contribute to mixture toxicity effects.</p> <p>Overall, the tasks of WG-1 are aimed to:</p> <ul style="list-style-type: none"> Ensuring that all these layers of information are maintained and regularly updated to allow for assessment of chemical risks in a timely manner, thus enabling time risk management Integrating and exploiting all this information for identification of lists of chemicals in need of priority actions (each priority list corresponds to an action). <p>Description of the proposed activity and expected outcomes for 2022 (and beyond):</p> <p>Task 1: Support the prioritisation work of the Commission services at European level and comment on relevant documents and queries (PARC, EWS, where relevant).</p> <p>NORMAN has participated as a stakeholder in the WG Chemicals of DG ENV and intends to further contribute in the activities related with the review of the list of WFD Priority Substances and the Watch List.</p> <p>In 2021, NORMAN contributed to the EU Consultation for the review of the list of Priority Substances ("Impact Assessment of a possible revision of the lists of pollutants affecting surface and ground waters and the corresponding regulatory standards in the Environmental Quality Standards, Groundwater and Water Framework Directives"). In 2022, NORMAN aims to provide proposals for the 4th review of the Watch List. Moreover, NORMAN WG-1 will be able to contribute in the following new European initiatives:</p> <ul style="list-style-type: none"> PARC partnership with a particular focus on inventory of existing data and common knowledge on chemicals Identification of CECs of interest in the Early Warning System for Europe (DG ENV) Implementation of a Mixture Allocation Factor (MAF) to address mixture toxicity (on going Caracal process).

Task 2: Collection and compilation of compound-specific information in support of prioritisation

In 2020, efforts focused on the final harmonisation of the current raw ecotoxicity data to fit the revised NORMAN Ecotoxicology Database metadata requirements (derived 2019-2020). For this purpose, the DCT template had to be upgraded and the transformation tables were revised. At the end of 2021 - beginning of 2022, the harmonised data will be re-uploaded into the database to fit the new layout, e.g. regarding matrix and protection asset.

The work planned for 2020 and 2021 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 and will be postponed to 2022.

In 2021, the Ecotoxcentre has adapted their internal templates for data compilation to make direct transfer of raw data into the NORMAN ECOTOX Database as easy as possible. This has been tested on a set of substances and the corresponding data have already been uploaded to the NORMAN database further to approval by the Ecotoxcentre. This initiative can be pursued in 2022.

Task 3: PNEC derivation module

The module has been officially launched on the public website in 2021. At this stage, the functionality and the experimental and predicted PNEC entered in the NORMAN ECOTOX Database already allow for the prioritisation of about 65,000 substances.

The template for uploading existing PNEC/EQS from regulatory sources has also been revised and finalised. In 2020 a first batch of existing EQS have been compiled and uploaded for pesticides used in Switzerland (Ecotoxcentre), as well as Danish and Swedish EQS, as originally planned for 2020. Additionally, thanks to the application of the QSAR models (developed by UoA) it was possible to generate P-PNEC values for more than 30,000 additional NORMAN substances.

The upload file for existing PNEC will be revised to include MAC-EQS values as well as values for the marine environment, in order to allow the evaluation of marine monitoring data, as well as peak exposure concentrations, such as those resulting from the German small water body monitoring project. Moreover, new compartments, such as soil or sediments should be added in 2022 to extend the scope of the current prioritisation scheme to allow consideration of multiple lines of evidence from different compartments.

WG-1 will continue to promote and coordinate the participation of Ecotoxicity Experts to derive and approve (i.e. vote for) new or revised Lowest PNEC values for substances of the SusDat list, with a specific focus on substances that were highly prioritised in EU projects using the NORMAN Prioritisation Framework. The aim will be to replace predicted PNEC values for substances prioritised in Cat 3 and 5, by experimentally-based PNEC values, if feasible based on new data.

Task 4: Integration of a Mixture Risk Indicator

In 2021, WG1 started the discussion on the inclusion of mixture risks into the NORMAN Prioritisation Framework. For this purpose, 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 - should be introduced. This new index would be complementary to the existing Frequency of Exceedance (that only considers single compounds exceedances). In this way, e.g. compounds in Cat. 6 could be better distinguished to ensure that compounds are not overlooked. After a case study has been performed, a paper on the indicator will be published and it will be implemented into the prioritisation tool in 2022.

Task 5: Compilation of data / information regarding 'Use categories' and 'Chemical Functional Use' for all SusDat compounds

With the ever-growing number of NORMAN SusDat substances, it becomes inevitable to group them by 'Use category' and 'Chemical groups category'. The NORMAN Substance Factsheets already contain information retrieved from the US EPA Dashboard, but at present this is not sufficient to allow searching in the NDS by e.g., all pesticides, all herbicides; all pharmaceuticals, all antibiotics; or by, e.g. all PFAS, pyrethroids, PAHs, ionic surfactants. The classification of the compounds is not trivial, since each substance has often multiple uses and associated sub-classes. The different approaches applied for categorisation of the uses (e.g. by REACH, US EPA Dashboard, PubChem) are not fully harmonised. In the same context, categorisation of transformation products and their linkage to single / multiple parents is another challenge that NORMAN wants to address.

The collection of this information is crucial to the prioritisation work (e.g. identification of contamination sources for which actions are required, exploitation of lists of substances).

To achieve this objective, we propose to organise a strategy within WG-1 in line with the on-going collaboration between NORMAN and PubChem addressing the following sub-tasks:

- a) Finalise and approve the DCT template (as agreed on in the last WG1 meeting). This will require controlled vocabulary and a common understanding about "use categories" and "functional uses".

- We should aim at a harmonised classification for NORMAN.
- The DCT should be uploaded into a newly developed sub-module and should be used as an interface for experts to be able to interact online (to upload the information and amendments where needed). All changes made by the experts should be traceable. All the information (use and functional categories) will be directly linked and searchable from the Substances factsheets / SusDat and the prioritisation system.
 - Discuss in consultation with the WG what the best platform is to create a group repository for NORMAN to exchange expert views and establish harmonised "use" terms (e.g. Gitlab, Github page for the NORMAN network similar to MassBank consortium). Should the platform open to NORMAN members only? Or should it be open also to external experts? (LCSB^o)
 - The DCT is meant to be a living tool. The experts in WG-1 are invited to regularly review and upgrade the categories (e.g. add the mode of action) and harmonise the drop-down entries. Volunteers in WG1 will be appointed to be in charge of complex groups of compounds (e.g. all REACH or PFAS compounds) to suggest their categorisation.
 - Extraction of "Use" information from the various SLE lists (already available) and export of this information into PubChem (LSCB & PubChem Team) and into the DCT (citing SLE as the reference source). WG-1 members will help to prioritize the most relevant lists.
 - Pilot efforts to retrieve "Use" information from PubChem and other sources (e.g. Wikipedia, Wikidata, USEPA DashBoard, ChemSpider etc.) and integrate them into the Use category module. Translation tables will be created for each source to ensure harmonised entries compatible with the NORMAN Use category module. (LCSB, UBA, EI)
 - Programming the workflow resulting from the pilot efforts (cf. e) for the transfer of the information retrieved from PubChem and other sources into the Use category module (EI)

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 the application of the NTS workflow on the WW case study. The other studies planned in JPA 2021 – which could not be completed – will be postponed as listed below.

Test the prioritisation framework with NTS data on the following case studies (available datasets in EMPODAT + DSFP):

- Wastewater effluents: SOLUTIONS (12 WWTPs), JDS4 (11 WWTPs), UFZ JPA 2019, Germany (34 WWTPs), other European countries (to be finalised in 2022)
- Danube River Basin Specific Pollutants based on wide-scope target and suspect screening using JDS4 data (INERIS / EI)
- Black Sea Specific Pollutants based on wide-scope target and suspect screening using EMBLAS project data (UoA / EI)
- Prioritisation of contaminants in top predators and their prey using LIFE APEX project data (UoA / EI / UBA)

The aim will be in particular to study the overlaps of suspect screening results from the different case studies in the different compartments and to identify novel CECs to feed into the Early Warning System for Europe.

As regards the substances, NORMAN WG-1 will focus on EDCs, PFAS and PMT compounds in support of PARC and Green Deal projects.

Another action, already ongoing in 2021 and to be pursued in 2022:

- Identification of list of ranked SusDat chemicals relevant for acquisition of their chemical standards or MS(MS) information allowing for target screening. The list should be identified as a result of the prioritisation framework (suspects allocated to NTS Cat 4). The selection of such list of "most wanted" spectra will take into account the availability of information within the NORMAN SLE and other open resources such as PubChem and CompTox, and check which compounds are not in MassBank or other open spectral libraries already. Once purchased and measured, the data should become available on the NORMAN database system (e.g. MassBank, NORMAN-SLE) (UFZ, Eawag, LCSB).

Task 7: Prepare input to the Early Warning System for Europe (EWS) (to be pursued in 2022)

Based on the results of task 6, a proposal for an "EWS-signal" should be discussed and prepared. In this way, NORMAN can contribute and potentially define the format of these signals and become a backbone of this important EU strategy.

As part of the constant evolution of the NORMAN Prioritisation Framework we also intend to extend the coverage of environmental compartments feeding the prioritisation scheme (holistic view of chemicals in the environment).

Task 8: Lessons learnt from the case studies: improving the features of the prioritisation tool (consultation and programming activities)

	<p>An expert consultation within WG-1 will be organised to upgrade the interface and the features of the current on-line prioritisation tool.</p> <p>At the moment there is a set of parameters that can be defined before running the prioritisation (e.g. substance, country, year). There are also parameters that are automatically integrated in the queries (e.g. choice of the dilution factor when we perform the prioritisation on wastewater effluent datasets).</p> <p>Further additional features could be discussed. Some examples are given:</p> <ul style="list-style-type: none"> - Since we now want to extend the application of the prioritisation framework to other compartments and matrices (soil, terrestrial ecosystems, marine environment, etc.), it is useful to design the interface to automatically select the proper PNEC, depending on the matrix and the prioritisation objective. For example, if we want to prioritise contaminants in reclaimed water for reuse in irrigation, we might need to select the wastewater effluent datasets labelled as "reclaimed water / reuse irrigation" and match the concentration data with the corresponding PNEC_crop, specific for protection of human health. - We can also discuss the possibility of improving the "proxy pressures" metadata field in the current Data Collection Templates for the monitoring sites. This field is already included in the DCTs but it is not mandatory and it has rarely been filled in by the data suppliers. This metadata and the associated drop-down list could be revised by the experts based on the lessons learnt. This information is in fact very valuable for interpretation of the prioritisation results. - Integration of the Mixture Risk Indicator (MRI) in the interface. This is connected with the previous task (see Task 4) where we will define the integration of this new indicator in the overall scoring system of the prioritisation framework. - Options for the spatial visualisation of the prioritisation results. <p>This task will be organised in two steps:</p> <ol style="list-style-type: none"> 1) Meetings (virtual, if possible 1 physical meeting) for consultation of the WG-1 experts: proposals / desk work to revise the features of the prioritisation tool 2) Programming work: the programming work is expected to start in the second part of the year 2022 after agreement with the WG-1 experts, based on dedicated instructions derived by a smaller team of experts (resources: an envelope will be set aside for possible expenditure in 2022, in line with the outcomes of the consultation within WG-1). <p>Task 9: State of the environment in Europe</p> <p>As a new task for WG 1, we would like to integrate the results of single substances risks at certain sites into a total effect, by mapping the concurrent occurrence of chemical contaminants in Europe, across compartments: e.g. how many compounds exceed the lowest PNEC at each site?; or what is the total mixture risk at each site? These might become new chemical indicators to measure progress of e.g. remediation measures and inform policy decisions (cf. pesticides indicator of the EEA). This would allow NORMAN to e.g. support the Zero pollution monitoring report of the EEA. Moreover, analysis of datasets regarding the minimum (most toxic compounds) compared to the total effect (mixture risk) might allow to derive an indication of a retrospective mixture allocation factor (MAF) in support of the COM EGD initiative.</p> <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> ▪ Support the preparation of the programme of activities of the PARC partnership, with particular focus on inventory of existing data and common knowledge on chemicals in order to identify gaps in data and anticipate future trends. ▪ Support the implementation of an Early Warning System for Europe (DG ENV) ▪ Support to DG ENV / JRC for the review of the list of WFD Priority Substances, the Watch List for surface water and the Watch List for groundwater. ▪ Support to other MS or RB if requested. ▪ Support prioritisation of CECs as Sea Specific Contaminants in the marine environment (OSPAR, HELCOM, MED POL, Black Sea Commission). ▪ Links with WG-5 for identification of priority contaminants in treated wastewater intended for reuse ▪ Links with WG on Soil and the Terrestrial environment for prioritisation activities. ▪ Link with NTS CWG, in particular as regards DSFP, SLE and the definition of a mechanism for updating the NORMAN List of emerging substances as top priority substances of SusDat. ▪ NORMAN MassBank: prioritisation of relevant compounds whose mass spectra are not yet included in the online repository MassBank.
Participants	INERIS, EI, UBA, Ecotoxcentre, UoA, LCSB (All WG-1 are welcome)

Proposed contribution	in-kind <p>Ecotoxcentre: Contribution of raw-data collection for Swiss EQS Dossiers, Compilation of existing national EQS and validation of NORMAN PNEC proposals.</p> <p>UBA: Compiling of single substances dossiers and a list of pesticide RAC values.</p> <p>INERIS: Coordination of the WG, pursue the work for the review of the prioritisation methodology and testing of the “revised methodology” on five case studies. Proposals for improvement from lessons learnt (Task 1, 5, 6, 8)</p> <p>EI: Testing of the “revised methodology” on five case studies. Contribution to Tasks 1, 7, 9.</p> <p>LECB: Extensive efforts associated with the NORMAN-SLE and related collaborations</p>
Contribution needed from NORMAN Association¹	<p>Task 1: Support the prioritisation work of the Commission services at European level and comment on relevant documents and queries (PARC, EWS, where relevant).</p> <p>Task 2: Collection and compilation of compound-specific information in support of prioritisation</p> <ul style="list-style-type: none"> - Collection and compilation (automated retrieval using script) of regulatory PNECs evaluated by ECHA for industrial chemicals (REACH) and Biocides including PNEC_{fw}, PNEC_{marine}, PNEC_{sed}, PNEC_{soil} and PNEC_{biota} (secondary poisoning); compilation of experimental data related to the derivation of the Hazard score (2,000 €) (EI, UBA) - Collection and compilation of regulatory threshold values derived by international authorities (e.g. US EPA, CCME, ANZECC and ARMCANZ...) for water reuse in agricultural irrigation. Conversion of PNEC_{soil} into Quality Targets in sewage sludge/sediment applied on soil for fertilisation. (DERAC (resources for this task are accounted for under WG-5) <p>Task 3: PNEC derivation module</p> <ul style="list-style-type: none"> - Coordination activity of Expert Group Ecotox / training course (UBA / Ecotoxcentre: 1,000€) <p>Task 4: Integration of a Mixture Risk Indicator (MRI)</p> <ul style="list-style-type: none"> - Development/programming of a new database functionality for automated calculation of MRI. (EI/UBA: 5,000 €) <p>Task 5: Compilation of data / information regarding ‘Use categories’ and ‘Chemical Functional Use’ for all SusDat compounds</p> <ul style="list-style-type: none"> - Organisation and harmonisation / Collection and compilation of data / information available on ‘Use categories’ and ‘Chemical Functional Use’. (LCSB: 3,000€ (not spent in 2021) - Programming the workflow resulting from the pilot efforts for the transfer of the information retrieved from PubChem and other sources into the Use Category module. (EI: 3,600 €) <p>Task 6: Prioritisation framework: follow-up activities to apply the new workflow across compartments and specific chemical groups</p> <ul style="list-style-type: none"> - EI: 3,000 € <p>Task 7: Prepare input to the Early Warning System for Europe (EWS) (to be pursued in 2022)</p> <p>Task 8: Lessons learnt from the case studies: improving the features of the prioritisation tool (consultation and programming activities)</p> <ul style="list-style-type: none"> - Update/programming of the prioritisation module bringing together target and suspect screening data. - Interface to automatically select the proper matrix- and prioritisation objective-related PNEC; integration of the MRI; design and update of the interface for spatial visualisation of the prioritisation results. (EI: 5,000 € envelope for possible expenditure in 2022, to be used in line with the outcomes of the consultation within WG-1) <p>Task 9: State of the environment in Europe</p> <ul style="list-style-type: none"> - Programming of the module and visualisation of the results (EI: 4,000) <p>Total net budget under JPA 2022: € to be confirmed</p>

¹ Please, provide here a transparent justification of the requested resources and of the in-kind contribution, thereby distinguishing between the costs associated with “person-months” for the organisation, the “travelling costs” for invited speakers and the costs for the logistics (e.g. meals, room rental etc.)