

Proposals for NORMAN Joint Programme of Activities 2022

Title	Update of NORMAN EMPODAT – SUSPECT Database to support prioritisation activities
Type of activity	Database development
Leader	Nikiforos Alygizakis, Jaroslav Slobodnik (EI), Nikolaos S. Thomaidis (NKUA-National and Kapodistrian University of Athens), Valeria Dulio (INERIS) in cooperation with experts of WG1 and NTS CWG
Topic / activities	<p>Background / Justification for the proposed activity:</p> <p>The main mission of the NORMAN Association is to act as an interface between science and policy. To fulfil this mission, the identification and prioritization of emerging contaminants is essential. Information on thousands of contaminants and their risk, hazard and exposure characteristics is stored in the NORMAN Database System (NDS). NORMAN Digital Sample Freezing Platform (DSFP) is one of the NDS modules, which is used for archiving, processing, analysing, data mining and retrieving information from high-resolution mass spectrometry (HRMS). During the last years, DSFP has been enriched with numerous datasets from various campaigns such as the monitoring of river basins (e.g. Danube, Dnieper, Dniester, Siverskiy Donets rivers), Seas (e.g. Black Sea, Baltic Sea, Mediterranean Sea, North-East Atlantic), wastewater and biota (e.g. top predators and their prey across Europe within EU LIFE APEX; OSPAR CONnECT, UBA-HELCOM projects, etc.). All these HRMS datasets can be revisited in a fully automated and reproducible manner in order to retrieve information about the semi-quantitative occurrence of contaminants of emerging concern employing retrospective suspect screening workflow. The systematic retrieval of occurrence data of all compounds in the NORMAN Substance Database in samples archived in DSFP can be used in the WG1 (target & suspect data) prioritization scheme.</p> <p>The upgraded prioritization scheme has firstly been tested in 2019 and applied at its full potential after overcoming various challenges in 2021. The full automatization of the prioritization scheme is of utmost importance. The prioritization exercise of 2021 was conducted in an automatic manner for target screening data (https://norman-data.eu/nds_full2) and in a semi-automatic manner for suspect screening data. This exercise was valuable to provide the needed guidance for programming of the prioritization module. To achieve full automatization, a new NDS module named “EMPODAT – SUSPECT Database” (https://www.norman-network.com/nds/suspect/) was designed and programmed. 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 scheme and any other purposes. The outcomes of EMPODAT – SUSPECT Database are supposed to be an important building block of the European Early Warning System for chemical pollution in the environment.</p> <p>Description of the proposed activity and expected outcomes for 2022 (and beyond):</p> <p>The activity has been divided in the following tasks:</p> <p>Task 1: Upgrade of the new NDS EMPODAT – SUSPECT module based on the needs of WG1 and NTS CWG</p> <p>Task 2: Retrospective suspect screening on all available DSFP datasets (>2,500) to cover the widest possible spatial, temporal and matrix distribution</p> <p>Task 3: Import of the suspect screening results obtained by DSFP workflow in the EMPODAT - SUSPECT</p> <p>Task 4: Retrieval of information from EMPODAT – SUSPECT to feed the prioritization module based on the experience from the pilot exercise and DSFP screening output</p> <p>Task 5: Invitation of WG1&NTS CWG experts to rigorously evaluate the prioritization output and the interfaces</p> <p>The activity was proposed in 2021 and additional tasks are planned for 2022. If successful, it will be proposed to become a permanent activity of the NORMAN network.</p> <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> WG 1 Prioritisation Cross-Working Group Activity Non-target Screening (NTS) Improvement of NORMAN Digital Sample Freezing Platform Development of suspect screening workflows New module in the NDS Proposal of new substances to be uploaded into MassBank Europe
Participants	EI, UoA, INERIS, and all interested members of WG1 and NTS CWG
Proposed in-kind contribution	Working hours for implementation of tasks 2 and 5 (EI, UoA, INERIS) and overall coordination of the activity (EI).



Contribution needed from NORMAN Association¹	<p>Task 1: EI; 5,000 € - <i>Upgrade of the new NDS module based on the needs of WG1 and NTS CWG</i></p> <p>Task 3: EI / NKUA 1,800 € - Curation and upload of suspect screening data into the new NDS module.</p> <p>Task 4: EI / NKUA 3,200 - <i>Retrieval of information from EMPODAT – SUSPECT to feed the prioritization module based on the experience from the pilot exercise and DSFP screening output</i></p> <p><i>Total contribution required: 10,000 €</i></p>
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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.)