

Proposals for NORMAN Joint Programme of Activities 2023

Title	NORMAN Suspect List Exchange (NORMAN-SLE) https://www.norman-network.com/nds/SLE/
Type of activity	Website / service maintenance / development
Leader	Emma Schymanski (LCSB, Luxembourg)
Topic / activities	<p>Background / Justification for the proposed activity:</p> <p>The NORMAN Suspect List Exchange (NORMAN-SLE) is an initiative of the 2015 Joint Programme of Activities and is an established central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. The NORMAN-SLE and the compiled suspect list "NORMAN SusDat" have become the cornerstone/data basis for all NORMAN Database System (NDS) modules and prioritization efforts. Both have been very highly prioritized by members in recent JPAs. The split between NORMAN SusDat and NORMAN-SLE is primarily for logistical reasons (to clearly demarcate data gathering and delivery, the NORMAN-SLE, and the role of a substance database (NORMAN SusDat). The NORMAN-SLE activity involves the addition of new lists to the Suspect List Exchange, which can then feed into SusDat, which has become the chemical data basis behind all NDS modules. In 2022 we finally achieved a long-awaited milestone of publication of the NORMAN-SLE, with 97 co-authors from 58 institutions (DOI: 10.21203/rs.3.rs-1902466/v1).</p> <p>As NORMAN-SLE is gaining increasing attention as an expert knowledgebase with high potential for greater impact, some additional resources are again requested this year to help curate and add necessary lists already identified as critical gaps (increase coverage, including transformation products), to work towards a more sustainable model following FAIR principles and allowing direct and automated (as far possible) integration into international resources. We are also working very closely with PubChem and the InChI Trust on UVCB, mixture and transformation product data management.</p> <p>Description of the proposed activity and expected outcomes for 2023:</p> <p>In 2023 we plan to continue and expand on the efforts from recent years, including:</p> <ul style="list-style-type: none"> • Website maintenance and development • Addition of new lists from external contributors when they become available • Addition of new lists strategically selected to fill identified knowledge gaps • Addition of lists to specifically save/register/link transformation product information • Archiving of all datasets on Zenodo (https://zenodo.org/communities/norman-sle) • Deposition of all substances in PubChem • Integration of lists into PubChem [on hold indefinitely: integration of lists into CompTox Chemicals Dashboard] • Progressive addition of annotation content to PubChem to fill information gaps • Extension and development of Transformations functionality with PubChem, both in terms of datasets and integration into workflows • Continuing development of new strategies to deal with UVCBs • Further development of strategies to deal with tentative/unknown/related structures • Publication(s) on ideas and methods behind Suspect List Exchange (biannual, revisit 2024?) • Open software/packages/approaches for curation/merging once appropriate (in close collaboration with SusDat (see SusDat proposal) <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> • The Suspect List Exchange will feed SusDat, the chemical source for other NDS modules • MassBank and the Suspect List Exchange are cross-linked • The Digital Sample Freezing Platform, Retrospective Screening and NormaNEWS • Prioritization working group • Various other activities within Cross-Working Group Activity NTS • Integration of NORMAN substances, annotation content, classification browser into PubChem is supporting the development of future NTS tools (e.g. PubChemLite, Classification browsers) • Considerable overlap with ELIXIR activities, especially ELIXIR-Toxicology community • NORMAN-SLE is a key element in the PARC initiative, the ZeroPM project and several and other EU initiatives
Participants	LCSB, EI, other interested parties and contributors; in co-operation with Evan Bolton and team (PubChem)
Proposed in-kind contribution	LCSB: coordination of upload of new lists to the website, basic maintenance, promotion EI: website updates and maintenance, coordination with SusDat PubChem, CompTox: time and resources associated with integration efforts Other partners: contribution of lists and ideas
Contribution needed from NORMAN Association¹	LCSB: partial costs associated with additional staff for addition / processing of new lists highly relevant for NORMAN and development of SLE-related codebase and infrastructure: €9000 [3 months 50 % R&D specialist salary, remaining 9 months covered by internal budgets]

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.)