

Proposals for NORMAN Joint Programme of Activities 2022

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| 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>As part of a series of workshops in September 2014, NORMAN members expressed the need to exchange various lists of substances to improve their suspect screening efforts. An initiative of the 2015 Joint Programme of Activities involved establishing the Suspect List Exchange as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. As part of the Databases meeting in Berlin, 2016 it was decided by members that the Suspect List Exchange and the compiled suspect list "SusDat" would become the cornerstone/data basis for all NORMAN Database System (NDS) modules and prioritization efforts and the Suspect List Exchange activity was very highly prioritized by members in the 2018 JPA. In 2019, the Suspect List Exchange (NORMAN-SLE) and NORMAN SusDat activities were split – SusDat is now covered in a separate activity. Since this time, both are consistently rated high priority activities by members. This 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. 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) and also work towards a more sustainable model following FAIR principles and allowing direct and automated (as far possible) integration into international resources.</p> <p>Description of the proposed activity and expected outcomes for 2022:</p> <p>In 2022 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 • Progressive addition of annotation content to PubChem to fill information gaps • Extension and development of Transformations functionality with PubChem, both in terms of datasets and integration into workflows • Integration of lists into PubChem and CompTox Chemicals Dashboard • Development of new strategies to deal with UVCBs • Further development of strategies to deal with tentative/unknown/related structures • Publication(s) on ideas and methods behind Suspect List Exchange • Open software/packages/approaches for curation/merging once appropriate <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 • The linking of the CompTox Chemicals Dashboard and the Suspect Exchange is win-win for both and increases visibility for both efforts (many access our lists through CompTox) • 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 • Great interest in NORMAN-SLE in the PARC initiative and other EU initiatives |
| Participants | LCSB, EI, other interested parties and contributors; in co-operation with Evan Bolton and team (PubChem) plus Antony Williams (US EPA) |
| 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.)