

Proposals for NORMAN Joint Programme of Activities 2022

Title	Update and improvement of the NORMAN Substance Database
Type of activity	Database development
Leader	Nikolaos S. Thomaidis (NKUA-National and Kapodistrian University of Athens), Jaroslav Slobodnik (EI-Environmental Institute)
Topic / activities	<p>Background / Justification for the proposed activity:</p> <p>Since the development and introduction of NORMAN Substance Database (SusDat; https://www.norman-network.com/nds/susdat/) in 2016, it benefited numerous activities of the network. SusDat is at present globally well recognised compound database of environmentally-relevant contaminants of emerging concern (CECs). Currently, it contains over 106,000 compounds accompanied with essential information on their unique chemical identifiers, chemical curation level, adduct forms, chemical properties, Retention Time Index (RTI). QSAR-predicted no-effect concentrations (P-PNECs), Use Category information, etc. SusDat is at the core of many other database modules in the NORMAN Database System (NDS; Digital Sample Freezing Platform (DSFP), EMPODAT, Ecotoxicology Database, Substance Factsheets and Passive Sampling Database). SusDat is a source database of DSFP and the new NDS module EMPODAT-SUSPECT, which are now directly feeding updated NORMAN Prioritisation Framework. It is also the most frequently visited module of the NDS. A continuous update, maintenance and improvement of quality of information in SusDat is of importance for the NORMAN network..</p> <p>This proposal aims to continue with systematic (i) upload of individual substance lists contained in the Suspect List Exchange (SLE), (ii) their merging and chemical curation, and (iii) adding missing and new information.</p> <p>Description of the proposed activity and expected outcomes for 2022 (and beyond):</p> <p>Task 1: Addition of <i>in-silico</i> predicted Retention Time Index (RTI) values for electrospray ionization (both positive and negative) and P-PNECs for all substances in SusDat.</p> <p>Task 2: Update of RTIs and P-PNECs for substances with updated chemical structure.</p> <p>Task 3: Application of an automated curation workflow developed in previous years to update the <i>validation level</i> for all substances. Adding missing <i>validation level</i> information for newly added substances.</p> <p>Task 4: Addition of qualifier fragment ions.</p> <p>Task 5: Addition of critical chemical identifiers.</p> <p>Task 6: Addition of preferable analytical methods for each compound (i.e. GC-EI, LC-(-/-)ESI etc.).</p> <p>Task 7: Investigation of potential deployment of the automated curation workflow.</p> <p>Task 8: Addition of toxicity threshold data for terrestrial environment and human health.</p> <p>Task 9: Addition of consensus models for logBCF, logK_{oa}, logK_{oc} and logK_{ow}</p> <p>Task 10: Addition of ionization efficiency (logIE) values.</p> <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> - Integration in Cross-Action Working Group CTS. - Integration in NORMAN Digital Sample Freezing Platform. - Interlink with other working groups within NORMAN - Interlink with WG1 Prioritisation.
Participants	Any interested parties
Proposed in-kind contribution	<p>EI: Integration of all new data/information in SusDat and Task 6</p> <p>UBA: Evaluation of the quality of toxicological data</p> <p>NKUA: Tasks 5, 8, 9, 10</p>
Contribution needed from NORMAN Association	<p>Task 1, 2, 3, 5, 6, 8, 9, 10: NKUA 4,000 €</p> <p>-Addition of properties for newly added compounds</p> <p>Task 4: NKUA 2,000 €</p> <p>- Addition of qualifier fragment ions</p> <p>Task 7: EI / NKUA 6,000 €</p> <p>- Programming of the interlink between SLE and SusDat</p> <p>- Improvement/programming of the automated curation algorithm for removal of duplicates (names, CAS Nos., InChIKeys) and manual check/curation of the flagged 'problematic' compounds</p> <p><i>Total contribution required: 12,000 €</i></p>