Proposals for NORMAN Joint Programme of Activities 2023

Title	**NORMAN MassBank / RMassBank**
Type of activity	Databases development
Leader	Tobias Schulze (UFZ Leipzig) and Emma Schymanski (LCSB Luxembourg) in co-operation with Steffen Neumann (IPB Halle) and Michael Stravs (Eawag)
Topic / activities	***Background / Justification for the proposed activity:*** - Continuous development and upgrade of NORMAN MassBank and related activities ***Description of the proposed activity and expected outcomes for 2023:*** - Upload of mass spectra to MassBank. All NORMAN members are welcome to contribute! - Further development of RMassBank - Further development of MassBank server platform (e.g. database and applications programming interface, curation of records, import and export of records, standardisation of curation rules) - Fostering the integration of MassBank with other mass spectral and metadata platforms (e.g., MoNA, PubChem, GNPS, US EPA CompTox, NORMAN SusDat) - Fostering the discussion with vendors for better integration of vendors' software with MassBank - Continuing the discussion on prioritised compounds missing in MassBank (matches to SLE, priority mixtures etc.). - Establishment of a chemicals' exchange platform to share neat standards for the creation of MassBank records and confirmation of identified compounds - Making MassBank more FAIR (e.g. better integration of ontologies, linked to NFDI4chem) - Integration of MassBank in NFDI4chem as central repository (2020-2025) - Evaluation of the MassBank data with regards to 1) chemical space covered and 2) reproducibility of spectra between groups and instrument types - MassBank training workshop in Q1/2023 ***Added value / Link with other NORMAN activities and / or other projects*** - Enhancement of non-target identification tools and workflows - Integration with PubChem and CompTox Dashboard, including fragment list - NORMAN Digital Sample Freezing Platform relies on the fragment information - Cross-Action Working Group NTS. - Integration into PubChem - Interaction with NFDI4chem - Bridging to WG1 Prioritisation
Participants	UFZ, LCSB, UoA, IPB Halle, Eawag, other interested parties
Proposed in-kind contribution	UFZ: Hosting and maintenance of MassBank Europe server, programming of RMassBank, issue input to MassBank platform development; fostering discussions on priority compounds for MassBank and implementation of a platform for exchange on most wanted mass spectra and collect volunteers. LCSB: compilation of MS records; issue input to MassBank platform development; contact to MoNA, PubChem, CompTox etc. Eawag: Programming and maintenance of RMassBank, compilation of MS records. IPB: Consulting of whole project, MassBank platform development, involving in making MassBank more FAIR and integration of MassBank in NFDI4Chem MassBank consortium: Further development of MassBank server platform NFDI4chem: Further development of MassBank server platform, integration as core repository in NFDI4chem, contact to vendors
Contribution needed from NORMAN Association[1]	Contribution of new mass spectra and issues for MassBank development; and all other inputs for enhancement of the MassBank environment

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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.)