



## Proposals for NORMAN Joint Programme of Activities 2022

<b>Title</b>	<b>MassBank Europe / RMassBank / Priorization of compounds for MassBank</b>
<b>Type of activity</b>	Databases development
<b>Leader</b>	Tobias Schulze (UFZ Leipzig), Emma Schymanski (LCSB Luxembourg), Michele Stravs (Eawag) in co-operation with Steffen Neumann (IPB Halle) and NFDI4Chem
<b>Topic / activities</b>	<p><b>Background / Justification for the proposed activity:</b></p> <ul style="list-style-type: none"> <li>- Continuous development and upgrade of MassBank Europe and related activities</li> </ul> <p><b>Description of the proposed activity and expected outcomes for 2022:</b></p> <ul style="list-style-type: none"> <li>- Upload of mass spectra to MassBank (UFZ, Eawag, LCSB - all NORMAN members welcome!)</li> <li>- Maintenance of RMassBank               <ul style="list-style-type: none"> <li>o improve input of peak list-based data</li> <li>o integrate mzTAB + MGF input (e.g. as export from pre-processing in other software)</li> <li>o integrate JCAMP input and workflow (e.g. Agilent PCDL exported libraries)</li> <li>o maintenance and update of existing functions</li> </ul> </li> <li>- Maintenance of the MassBank server platform               <ul style="list-style-type: none"> <li>o maintenance and update of existing functions</li> <li>o implement a new spectral search function</li> <li>o improve the representation of mass spectra and structures to be more interactive</li> </ul> </li> <li>- Maintenance of MassBank data               <ul style="list-style-type: none"> <li>o maintenance and update of curation functions</li> <li>o integration with PubChem (update annotation, deposition in PubChem, CIDs in MassBank)</li> <li>o implement more consistent display of chemical identifiers (e.g. preferred MassBank name)</li> <li>o a FAIRer presentation of the records (e.g. implement author tags)</li> <li>o integration of UOA RTI and ionization efficiency</li> </ul> </li> <li>- Foster and maintain interoperability with global partners               <ul style="list-style-type: none"> <li>o NFDI4Chem, PubChem and others</li> <li>o Integration of MassBank in NFDI4Chem as central repository (2022-2025)</li> </ul> </li> <li>- Prioritization of chemicals for upload               <ul style="list-style-type: none"> <li>o Fostering the discussion on prioritised compounds missing in MassBank (matches to SLE, priority mixtures etc.), create a list of most wanted spectra and establish a platform for exchange of information.</li> <li>o Establishment of a chemicals' exchange platform to share neat standards for the creation of MassBank records and confirmation of identified compounds.</li> <li>o Evaluation of MassBank data in regards to 1) chemical space covered and 2) reproducibility of spectra between groups and instrument types.</li> </ul> </li> <li>- Training and demonstration               <ul style="list-style-type: none"> <li>o Organize an online workshop on RMassBank processing and downstream analysis using MassBank spectra</li> </ul> </li> </ul> <p><b>Added value / Link with other NORMAN activities and / or other projects</b></p> <ul style="list-style-type: none"> <li>- Enhancement of non-target identification tools and workflows</li> <li>- NORMAN Digital Sample Freezing Platform relies on the fragment information</li> <li>- Cross-Action Working Group NTS.</li> <li>- Interaction with NFDI4chem, PubChem and other global partners</li> <li>- Bridging to WG1 Prioritisation</li> </ul>
<b>Participants</b>	UFZ, LCSB, UoA, IPB Halle, Eawag, other interested parties
<b>Proposed in-kind contribution</b>	<p>UFZ: Hosting and maintenance of MassBank Europe server, issue input to MassBank platform development; organization of an online MassBank workshop</p> <p>LCSB: Integration with PubChem, contribution to RMassBank, compilation of MS records; issue input to MassBank platform development; contact to MoNA, PubChem, CompTox etc.</p> <p>Eawag: Programming and maintenance of RMassBank, compilation of MS records, issue input to MassBank platform development.</p> <p>IPB: Consulting of whole project, MassBank platform development</p> <p>UoA: Integration of new RTI approaches into MassBank records</p> <p>MassBank consortium: Further development of MassBank server platform</p> <p>NFDI4chem: Further development of MassBank server platform, integration as core repository in NFDI4chem, contact to vendors</p>
<b>Contribution needed from NORMAN Association</b>	<p>Contribution of new mass spectra, neat standards, and issues for MassBank development.</p> <p>6000 € for R and/or Java programming and implementation of a platform for exchange on most wanted mass spectra and related neat standards.</p>