

## Proposals for NORMAN Joint Programme of Activities 2022

<b>Title</b>	<b>Development of QSIR models for Ion mobility spectrometry</b>
<b>Type of activity</b>	Database development; suspect screening, identification of unknowns
<b>Leader</b>	Nikolaos S. Thomaidis (NKUA), Nikiforos Alygizakis (NKUA/EI), Jaroslav Slobodnik (EI)
<b>Topic / activities</b>	<p><b>Background / Justification for the proposed activity:</b></p> <p>Hyphenation of ion mobility separation (IMS) to high resolution mass spectrometry (HRMS) has clear benefits for the identification of contaminants of emerging concern. IMS separates the ions based on their shape and size. The time taken for an ion to travel through a mobility device can be translated into its collision cross section (CCS). This value gives an overall estimation of the size of the sphere created by the ion when moving across a gas phase. IMS enhances the performance characteristics of LC-HRMS screening workflows by providing a new separation dimension (termed as 4D identification) and results in the drastic reduction of false positive identifications and separation of isomeric/isobaric compounds. IMS-HRMS provides many unexplored opportunities and it is expected to become mainstream in the next years. Until now, there are only few tools and databases available and there is a demand to create large libraries and robust QSIR approaches with <b>large applicability</b> domain and <b>declared uncertainty</b> and <b>high precision</b>.</p> <p>This proposal aims to enrich the NORMAN Database System with CCS values to support the suspect screening workflow integrated in Digital Sample Freezing Platform (DSFP) and other activities. The proposal includes the aggregation of experimental CCS values from literature, peer-review of models to predict CCS values and creation of robust QSIR models to predict CCS values for all NORMAN SusDat compounds.</p> <p><b>Description of the proposed activity and expected outcomes for 2022:</b></p> <ul style="list-style-type: none"> <li>- <b>Task 1:</b> Gather as many experimental CCS values as possible from literature and NORMAN laboratories</li> <li>- <b>Task 2:</b> Incorporation of the collected CCS in MassBank text records and in the Suspect List Exchange (SLE) lists</li> <li>- <b>Task 3:</b> Review modelling efforts from literature</li> <li>- <b>Task 4:</b> Based on the literature review, use of already existing models or creation of new models to predict CCS values for all SusDat compounds</li> <li>- <b>Task 5:</b> Creation of an API and a standalone web-based application for CCS value prediction to assure sustainability of SusDat</li> <li>- <b>Task 6:</b> Integration of CCS in the NORMAN Database System and upgrade of screening functionality of DSFP</li> </ul> <p><b>Added value / Link with other NORMAN activities and / or other projects</b></p> <ul style="list-style-type: none"> <li>- Improvement of non-target identification tools and workflows.</li> <li>- Integration in Cross-Action Working Group NTS CTS.</li> <li>- Integration in NORMAN Digital Sample Freezing Platform.</li> <li>- Interlink with other WGs within the NORMAN network.</li> <li>- Bridging to WG1 Prioritisation.</li> <li>- Enrichment of NORMAN SusDat via identification of relevant new isobaric/isomeric compounds in various matrices (e.g. indoor environment dust, biota, soil and (waste)water samples).</li> </ul>
<b>Participants</b>	NKUA, EI, UJI, UFZ, LUBW and all interested NORMAN members with ion mobility instruments. All members will be invited to participate.
<b>Proposed in-kind contribution</b>	<ul style="list-style-type: none"> <li>• All NORMAN members: Measurement of CCS values, compilation of experimental database, development of prediction models for CCS values of SusDat and development of web-based CCS tool with a CCS bank.</li> <li>• UFZ&amp;MassBank consortium: Integration of the information in MassBank records</li> <li>• LUBW: Integration of the information in SLE and PubChem</li> </ul>
<b>Contribution needed from NORMAN Association<sup>1</sup></b>	<p>Task 1: NKUA; 5,000 €</p> <ul style="list-style-type: none"> <li>- Literature review and compilation of CSS values</li> </ul> <p>Task 4&amp;5: NKUA; 5,000 €</p> <ul style="list-style-type: none"> <li>- Development of models, prediction of CSS for SusDat compounds and creation API and a standalone web-based application</li> </ul> <p>Task 6: EI; 2,000 €</p> <ul style="list-style-type: none"> <li>- Integration of CSS to DSFP search functionality</li> </ul> <p><i>Total contribution required: 12,000 €</i></p>

<sup>1</sup> 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.)