

Proposals for NORMAN Joint Programme of Activities 2023

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| Title | Collaborative Trial for the intercomparison of Ion mobility separation data. Development of open-access CCS databases for IMS. |
| Type of activity | Intercomparison of IMS data; Database development; suspect screening, identification of unknowns |
| Leader | Alberto Celma (SLU), Konstantina Diamanti (NKUA), Nikolaos S. Thomaidis (NKUA), Nikiforos Alygizakis (NKUA/EI), Lubertus Bijlsma (UJI), Jaroslav Slobodnik (EI), Teresa Steininger-Mairinger (BOKU) |
| Topic / activities | <p>Background / Justification for the proposed activity:</p> <p>The hyphenation of ion mobility separation (IMS) to high resolution mass spectrometry (HRMS) has shown clear benefits for the identification of contaminants of emerging concern in complex environmental samples. IMS separates ions based on their charge, shape and size. The time taken for an ion to travel through a mobility device i.e. drift time 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 it results in cleaner spectra, the reduction of false positive identifications, enhanced identifications, and potential separation of isomeric/isobaric compounds. IMS-HRMS provides many unexplored opportunities and it is expected to become mainstream in the next years. Therefore, there is a need to develop open-access databases for sharing IMS data among laboratories. To this purpose, the inter-instrument comparability of CCS values should be carefully assessed both for the obtained values and the instrument calibrants used. Special focus will be put on the selection of calibrants, since recent data indicates, that CCS values do depend on the ion mobility instrument as well as on the set of compounds used for calibration. Additionally, the development of universal QSIR approaches with large applicability domain is pivotal for the implementation of IMS-HRMS. This proposal aims to evaluate the comparability of CCS values between different instrumental configurations, enrich the NORMAN Database System with CCS values to support the suspect screening workflow integrated in Digital Sample Freezing Platform (DSFP) and develop a universal model for CCS values estimation. The proposal also includes the aggregation of experimental CCS values from participant laboratories, analysis of standards and creation of robust QSIR models to predict CCS values for all NORMAN SusDat compounds.</p> <p>Description of the proposed activity and expected outcomes for 2023:</p> <ul style="list-style-type: none"> - Task 1: Collect experimental CCS values from NORMAN participating laboratories both from already available data and also newly acquired data. - Task 2: Evaluate comparability of CCS values at both intra- and inter-instrument scale. - Task 3: Incorporation of the collected CCS in MassBank text records and in the Suspect List Exchange (SLE) - Task 4: Based on the literature review, use of already existing models or creation of new models to predict CCS values for all SusDat compounds - Task 5: Creation of an API and a standalone web-based application for CCS value prediction to assure sustainability of SusDat. Incorporation of CCS to SusDat - Task 6: Integration of CCS in the NORMAN Database System and upgrade of screening functionality of DSFP <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> - Improvement of non-target identification tools and workflows. - Integration in Cross-Action Working Group NTS CTS. - Integration in NORMAN Digital Sample Freezing Platform. - Interlink with other WGs within the NORMAN network. - Interlink with PubChem to populate CCS values |
| Participants | SLU, NKUA, EI, UJI, EAWAG, BOKU and all interested NORMAN members with ion mobility instruments. All members will be invited to participate. |
| Proposed in-kind contribution | <ul style="list-style-type: none"> • All NORMAN members: Measurement of CCS values • SLU, NKUA, EI, UJI, EAWAG, BOKU: compilation of experimental databases, development of prediction models for CCS values of SusDat and development of web-based CCS tool with a CCS bank. • UFZ&MassBank consortium: Integration of the information in MassBank records • LUBW: Integration of the information in SLE and PubChem |
| Contribution needed from NORMAN Association¹ | <p>Task 1-3: SLU; 5,000 €</p> <ul style="list-style-type: none"> - Compilation and evaluation of CCS values - Update of MassBank and SLE databases <p>Task 4&5: NKUA; 5,000 €</p> <ul style="list-style-type: none"> - Development of models, prediction of CCS for SusDat compounds and creation API and a standalone web-based application <p>Task 6: EI; 2,000 €</p> <ul style="list-style-type: none"> - Integration of CCS to DSFP search functionality <p style="text-align: right;"><i>Total contribution required: 12,000 €</i></p> |

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.)

