

Proposals for NORMAN Joint Programme of Activities 2026

Title	NDS-CCS: An open database for sharing ion-mobility derived collision cross section (CCS) values
Type of activity	Database development; Widen the application of IMS for the identification of unknowns; Share of data ensuring FAIR (Findability, Accessibility, Interoperability, Reuse) principles; Secure existing databases
Leader	Lidia Belova (UAntwerpen), Alberto Celma (SLU), Lubertus Bijlsma (UJI), Emma Schymanski (LCSB)
Topic / activities	<p>Background / Justification for the proposed activity:</p> <p>Hyphenating ion mobility separation (IMS) with high-resolution mass spectrometry (HRMS) has demonstrated clear advantages for the annotation of emerging environmental contaminants in complex matrices. IMS allows the separation of ions based on their shape, size and charge, and gaseous mobility resulting thereof. From the measured mobility, a collision cross section (CCS) value can be calculated for every analyte. The CCS value can serve as an additional annotation parameter for the identification of chemicals in suspect and non-target screening. The implementation of IMS in exposomics studies has shown a vast increase in recent years. However, the use of CCS values for compound annotation is dependent on the availability of open access databases providing reference CCS values, derived from reference standards or, if latter are not available, from prediction models. Numerous extensive datasets, both predicted and experimental, have been published and made available to the scientific community covering a wide range of environmental contaminant classes, their metabolites, endogenous compounds etc. To improve data accessibility, these CCS datasets can be gathered in open access repositories (e.g., NORMAN-SLE) or implemented in existing chemical databases such as PubChem. However, given the current political developments leading to substantial cuts in research funding and putting the accessibility of US based large scale data repositories at risk, there is a growing need to establish European datahubs to secure available CCS repositories and their availability to the scientific community.</p> <p>Therefore, this proposed joint programme activity aims at establishing a Europe-based database for the collection, consolidation and comparison of experimental reference CCS data. First, the datahub will be populated with experimental CCS data already consolidated within the NORMAN-SLE, PubChem, the dataset collected within the NORMAN JPA conducted in 2023 (a large dataset from 19 participating laboratories) and new relevant literature data. All data will be gathered in a newly created easily accessible webpage facilitating FAIR data sharing within the scientific community. The webpage will also ensure easy integration of new CCS datasets submitted by other NORMAN laboratories or external partners. To facilitate future data submissions, a data reporting template, with harmonized required experimental parameters to be included, will be developed. These actions will set the basis for further developments and improvement of CCS prediction data and establishment and wider implementation of experimental CCS-<i>m/z</i> trendlines for the annotation of homologue series of environmental contaminants.</p> <p>Description of the proposed activity and expected outcomes for 2026:</p> <ul style="list-style-type: none"> - Task 1: Collection of existing experimental CCS datasets from the NORMAN-SLE, NORMAN JPA 2023 on CCS inter-comparison, PubChem, and recent IMS studies in the exposomics field - Task 2: Consolidation of CCS data reporting to harmonize available experimental parameters including instrumental set-up, calibration approach, measurement parameters, etc. - Task 3: Creation of an open source webpage for CCS data sharing, interlinking compound data with PubChem and SusDat databases - Task 4: Development of a standardized procedure for submission of experimental reference CCS datasets by NORMAN and external partners including minimum requirements of needed information <p>Added value / Link with other NORMAN activities and / or other projects</p> <ul style="list-style-type: none"> - Preservation of open access data and their accessibility for the scientific community - Interlink with SusDat database - Integration in Cross-Action Working Group NTS CTS - Interlink with other WGs within the NORMAN network
Participants	UAntwerpen, SLU, UJI, LCSB, and all interested NORMAN members with ion mobility instruments. All members will be invited to participate.
Proposed contribution	<p>in-kind</p> <ul style="list-style-type: none"> - All NORMAN members: Possible contribution of CCS datasets - UAntwerpen, SLU, UJI, LCSB: Collection and consolidation of CCS datasets, development of standardized procedure for data submission, database expansion - UAntwerpen, LCSB: Webpage development
Contribution from Association¹	<p>needed NORMAN</p> <p>Task 1-2 & 4: UAntwerpen, SLU, UJI, LCSB: 2,000 €</p> <ul style="list-style-type: none"> - Collection/consolidation of CCS data, submission template development - Distribution of materials between NORMAN partners <p>Task 3: UAntwerpen, LCSB: 10,000 € (1.5 months technical support and/or 7 months student assistance)</p> <ul style="list-style-type: none"> - Development of open access webpage for data sharing and collection

Total contribution required: 12,000 €

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.)