



## Invitation to:

# NORMAN Collaborative Trial 2023-2024

**Intercomparison of Ion mobility separation data.**

**Development of open-access CCS databases for IMS.**

This Collaborative Trial is organized by the NORMAN Association as part of its Joint Program of Activities for the year 2023-2024. The activity is an initiative within the Cross-Working group in Non-target screening (NTS), although members from other working groups are also invited to take part on.

The Collaborative Trial is a joint initiative by Swedish University of Agricultural Sciences (SLU), National and Kapodistrian University of Athens (NKUA), Environment Institute (EI), University Jaume I (UJI) and University of Natural Resources and Life Sciences (BOKU). These institutions will be responsible for the scientific and technical preparation of the exercise, the collection, evaluation and dissemination of the results, in cooperation with trial participants.

### **Background**

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.



## **Objectives**

The main objective of this collaborative trial is to evaluate the comparability of CCS values between different instrumental configurations permitting thus the use of third-party laboratory data in tentative identifications in suspect and non-target screening. For that, we pursue the following detailed objectives:

- Assessment of the comparability of CCS data among different instruments, or same instruments using different conditions.
- Enrichment of the NORMAN Database System with CCS values to support the suspect screening workflow integrated in Digital Sample Freezing Platform (DSFP).
- Development of a universal model for CCS values estimation.

## **Work plan for the trial**

The Collaborative Trial will be performed at different steps as follows:

1. Collection of already available online and in-house CCS databases from the participant laboratories(\*) to evaluate already available data as well as being included in step 4. (\* Only for labs who willingly want to share this data, not compulsory)
2. Identification of needs for specific substances to be included in the trial based on availability of data in databases.
3. Distribution of reference standards (mix solution) among the participating laboratories to measure experimental CCS values.
4. Comparison of CCS values among different instrumental set-ups.
5. Incorporation of collected CCS values in MassBank text records and in NORMAN-SLE.
6. Prediction of CCS values for SusDat substances with either already existing or newly developed prediction models.
7. Creation of an API and a standalone web-based application for CCS values prediction to assure sustainability of SusDat. Incorporation of CCS to SusDat.
8. Integration of ion mobility in the NORMAN Database System and upgrade of screening functionality of DSFP.

Participation of NORMAN members is needed for measuring CCS values with their instrumental set-ups and providing already acquired data. All other activities will mainly be conducted by organizing team.

An **evaluation/discussion workshop** will most probably be organised in the beginning of 2024 to provide in-depth discussions of the results with the participating laboratories and plan future steps.

## **Timing**

The standard mixture to inject in LC-IMS-HRMS instruments is expected to be shipped in September-October 2023.



## **Reporting of results**

Results from each participant should be registered in an Excel reporting template which will be distributed to all participants. The template with the results should be returned electronically by **30<sup>th</sup> November, 2023**.

## ***Time schedule***

15 June 2023: Deadline for registration to the Collaborative Trial.

June-July 2023: Collection of in-house databases.

September-October 2023: Distribution of standard mixture among participants.

30 November 2023: Deadline for submission of the results by the participants.

March 2024 (date to be confirmed): Workshop about observed results.

## ***Participation and registration***

If you wish to participate, please **register [here](#)** before **June 15<sup>th</sup>, 2023**.

## **Participants**

Any laboratory equipped with LC-IMS-HRMS for the analysis of unknown organic pollutants (i.e. performing non-target screening) is invited to participate in this Collaborative Trial. Participation of external laboratories, i.e. non-NORMAN members, is very much welcome.

Participation includes reception of analytical reference standards, analysis in LC-IMS-HRMS instruments, submission of data regarding the instrumental set-up and the conditions (e.g. calibration) used, submission of the measured CCS values, and optional presence in the workshop about observed results.