Ion Mobility-High Resolution Mass Spectrometry for Screening of Contaminants of Emerging Concern (CECs) in Environmental Applications

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Ion mobility mass spectrometry (IM-MS) derived collision cross section (CCS) values can serve as a valuable additional identification parameter within suspect screening analyses of compounds of emerging concern (CECs), such as alternative plasticizers, organophosphate flame retardants, perfluoroalkyl chemicals and many others. However, their application for compound identification requires the availability of reference databases of CCS values which can be matched with experimental data. The unavailability of database values for many CECs and their metabolites hampers compound identification in environmental and human samples.

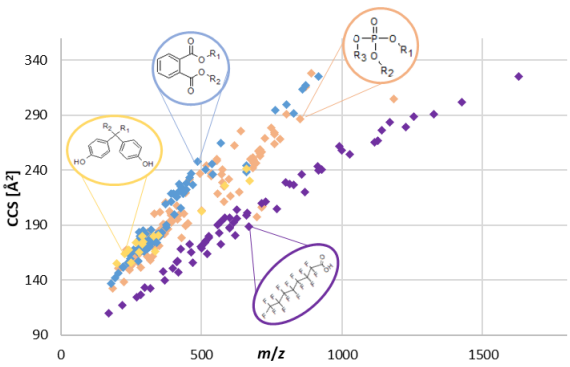

Figure 1. Depiction of $^{DT}CCS_{N2}$ vs *m/z* for the 148 CECs included in the database. The main compound classes are indicated: bisphenols (yellow), organophosphorus flame retardants (orange), plasticizers (blue), PFAS (purple).

To fill this knowledge gap, reference $^{DT}CCS_{N2}$ values of 148 CECs and their metabolites were acquired. Comprehensive quality assurance guidelines were implemented in the workflow of acquiring the $^{DT}CCS_{N2}$ values to ensure reproducible experimental conditions. For 105 compounds, more than one ion is reported yielding a database containing $^{DT}CCS_{N2}$ values for 311 ions obtained in positive and negative ionization polarities. The obtained dataset allows the characterization of trends observed for the CCS-*m/z* relationships of the investigated classes of CECs (Figure 1) and can serve as a valuable tool in suspect screening studies on CECs. Additionally, IM-MS allowed the separation of several commonly occurring isomers of some organophosphate flame retardants, plasticizers and their metabolites.

A suspect screening method for the screening of plastics' samples was developed coupling liquid chromatography to IM-MS. The obtained IM-MS data was matched against the developed $^{DT}CCS_{N2}$ database as well as previously published CCS databases aiming to characterize additives present in plastics which might be missed by commonly used target methods.