

Ion Mobility Spectrometry-Mass Spectrometry Workshop Report
Ion Mobility Spectrometry: What's next?

Wednesday, June 8th, 2022
Minneapolis Convention Center

Presiding: Kelly Hines (UGA) and Xueyun Zheng (PNNL)

For the ASMS 2022 IMS/MS workshop, we invited a panel of IMS/MS researchers to share their perspectives and forecasts for next major developments in the field. The presiders gave a brief introduction to the history of IM technologies and the release of commercial IMS/MS platforms. Each of the seven panelists gave a brief presentation on their recent work in IMS/MS and their thoughts on the future directions of IMS/MS. Prof. Thomas Rizzo (EPFL) spoke on the combination of ion mobility with infra-red spectroscopy and multiplexed IMS for carbohydrate identification and complex analyses. Prof. Christian Bleiholder (FSU) presented on their development of tandem trapped ion mobility (tTIMS) and tTIMS coupled with UVPD for top-down proteomic applications. Thomas Walker (Texas A&M) discussed the implementation of Fourier transform multiplexing to couple drift tube IMS with orbitrap mass analyzers. Prof. Gabe Nagy (Utah) spoke on the implications of mass distribution shifts from heavy isotopes on the separation of isotopomers with high-resolution cyclic IMS. Prof. Christopher Chouinard (FIT) presented on their strategy to use covalent derivatization methods to enhance structural separations of isomeric steroids with IMS. Prof. Facundo Fernández shared the work of his group to develop machine learning and quantum mechanics approaches for the prediction of collision cross section (CCS) values for metabolomics applications. Dr. Aivett Bilbao (PNNL) presented new software tools and algorithms for the visualization and processing of IMS/MS data.

The final 15-20 minutes of the workshop were used for discussion/Q&A with session's panelists. The need for normalization of CCS values between platforms and laboratories prompted an active discussion and several strategies were proposed, including the use of a relative CCS strategy similar to that used for calculating molecular weights relative to carbon (12 amu).

The workshop was very well-attended. We estimate that more than 100 attendees were present in the full room.