

**Ion Mobility-Mass Spectrometry Workshop:
From Data to Structure**
Wednesday, June 7th, 2023
George R. Brown Convention Center, Houston, TX

Presiding: Jim Prell (University of Oregon) and Xueyun Zheng (PNNL)

The ASMS 2023 Ion Mobility Workshop focused on different modern approaches to computing collision cross sections (CCS), from those that simulate the physics of the ion-gas scattering process to those that employ Machine Learning algorithms based on databases of experimental data. The presiders gave a brief introductory tutorial on ion mobility spectrometry and the challenges inherent in deriving structural information from a single number (i.e., CCS), as well as modern approaches to predict collision cross sections from molecular structures. Dr. Heiko Neuweiger (Bruker Daltonics) presented a talk on CCS-Predict Pro software and its performance in predicting small molecular ion CCS using experimental databases and Machine Learning. Prof. Carlos Larriba-Andaluz (IUPUI) then spoke about IMoS 2.0 software, which predicts ions' CCS by atomistically simulating buffer gas scattering as the ions traverse an ion mobility cell. Prof. Christian Bleiholder (Florida State University) gave a presentation about the Structure Relaxation Approximation, in which Molecular Dynamics simulations of ion structure relaxation on the gas-phase potential energy surface are combined with Projection Superposition Approximation computations of CCS to predict CCS distributions. A fourth talk by Prof. Steffen Lindert (The Ohio State University) discussed software developed by his group that combines Deep Learning algorithms (Rosetta and AlphaFold2), experimental ion mobility data, and Projection Approximation computations to predict solution-phase structures of biomolecules.

These talks were followed by a 20-minute Q&A with the speaker panel. Audience questions covered topics from remaining challenges in interpreting CCS in terms of structure to the need for larger, standardized repositories of experimental CCS data.

Workshop attendance was ~100 people.