

## Ion-Mobility Mass Spectrometry: Shooting Proteins into a Buffer Gas

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Abstract: Ion Mobility-Mass Spectrometry (IM-MS) is becoming an increasingly popular and powerful tool to investigate structure, conformational dynamics, and folding properties of proteins and other biomacromolecules. In short, an IM-MS experiment separates molecular ions of arbitrary shapes and sizes (ranging from small molecules up to megadalton protein complexes) based on their differential mobility through a buffer gas. Measurement of the molecule's time-of-flight through the drift chamber is readily related to the rotationally-averaged collisional cross-section of the target molecule with the buffer gas, from which valuable information can be extracted regarding its structural features. In this talk, I will present a detailed view of the molecular processes that take place in an IM-MS experiment from the structural perspective of the protein using Molecular Dynamics simulations. I will also show how the cross-section can be effectively computed from simulations and compared to experimental data.

**Key-words**: Ion Mobility-Mass Spectrometry, Collision Cross Section, Molecular Dynamics Simulation

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