Ion Mobility Investigations of Carbohydrate:Protein:Metal Non-Covalent Complexes

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Ion Mobility MS can be used to investigate changes in conformation of various biological molecules. This presentation will focus on how both arrival time distribution and collision cross section changes when metal ions and other ligands non-covalently coordinate to proteins. Electrostatic interactions and metal ion coordination cause proteins to shift from elongated to more compact structures. Chemotactic proteins MCP1 and MCP2 show shifts to a more compact structure with ligand (oligosaccharide and Ca^{2+}) binding. Shifts to a more compact or more elongated structure also occur depending on the radial and axial distance of the nanospray tip to the cone. While the MCP-1 dimer exhibited an unfolded structure at high collision energy in the trap cell of, the metal coordinated dimer exhibited a a more compact structure. Also observed was heparin octasaccharide, bound to MCP-1 dimer, which caused the formation of two ion conformation populations within the ion mobility spectrum.