ANALYTICAL SEMINAR

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"Exploring formation of protein ions in electrospray ionization"

Proteins play many important roles in biology with their structures affecting their function. Mass spectrometry (MS) is a valuable tool for analysis of these biomolecules. However, MS analyses require that these molecules be transferred from their biological, solvated states to gas-phase ions. Currently, charge-state distributions, collisional cross sections, ion activation, and soft landing are used to characterize the structures of gaseous ions. For proteins, the magnitude of a protein's charge in solution is dependent on the amino acid composition, which determines the isoelectric point (pI). Protein structure in the gas-phase is dependent on the amino acid composition and the ESI processes. Here, we present our ongoing efforts to examine how ESI charging affects gas-phase protein structures and stability using a combination of native MS, collision inducted unfolding, and molecular dynamics simulations.