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Solute-Solvent Structural Changes that Accompany Ion Dehydration in Electrospray Ionization (ESI) as Revealed by Cryogenic (80 K) Ion Mobility-Mass Spectrometry (IM-MS)[1]

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Peptide/protein conformer preferences are dictated by intra- and intermolecular interactions. Because of the large number of degrees-of-freedom in bulk solvent networks and the dynamic nature of hydrogen bonds, experimental studies of specific interactions of individual conformational states are difficult. Gas phase studies of solvent-free biomolecules provide a potential solution to this problem because inter- and intramolecular interactions are effectively decoupled. However, a potential concern is that during the transition from solution to gas phase the molecules encounter unique environments that can potentially affect their conformer preference. A number of studies have demonstrated that peptide/protein ions generated by ESI can retain memory of their solution structures, including retention of biological activity, suggesting that gaseous ions can be kinetically trapped in local minima along their potential energy surface owing to evaporative cooling and relatively slow rates of isomerization; however, the effect of charge state and extent to which non-covalent interactions are affected remains unresolved. Here, we discuss recent cryogenic (80 K) IM-MS studies that capture the evaporative dynamics of a series of model peptide ions. Cryogenic-IM affords new insights as to the multiplicity of peptide ion conformations and how solute-solvent interactions alter both solute and solvent structures.

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