FOLDAMERS, CROWNS, AND WATER: CONNECTIONS BETWEEN ISOLATED MOLECULES AND SOLUTION-PHASE BEHAVIOR

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This talk will provide an overview of recent results from our group that highlight the synergistic connections between single-conformation spectroscopy and laser-initiated isomerization data on isolated molecules and molecular clusters and issues of current interest to those studying solution-phase behavior. Single-conformation data in the C=O stretch region provide a foundation for those seeking to model 2D-IR data on polypeptides in solution. The infrared and ultraviolet spectra of size-selected crown-$(H_2O)_n$ and γ-peptide-$(H_2O)_n$ clusters reflect the ways in which first solvent shell water molecules interact with the binding pocket and H-bonding sites of these molecules. Infrared population transfer spectroscopy of the crown-water complexes will be used to probe energy flow between the water solvent and crown solute. Recent progress on methods that enable analogous studies on larger molecules will also be discussed.