WATER CLUSTERS OF TRYPTAMINE AND 3-INDOLEPROPIONIC ACID: THE ROLE OF WATER BRIDGES IN DIRECTING THE CONFORMATIONAL PREFERENCES OF FLEXIBLE BIOMOLECULES

BRIAN C. DIAN, JOEL R. CARNEY and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-1393*.

Resonant Ion Dip Infrared Spectroscopy, coupled with quantum chemical calculations, has been used to study water clusters of tryptamine (TRA) and 3-indolepropionic acid (IPA) in a jet-cooled molecular beam. We have seen in the case of TRA and IPA, that the monomers posse seven and two distinct conformational isomers, respectively. In TRA, past studies have shown that the addition of a single water molecule restricts its structure to a single conformation. Whereas in the case of IPA, the addition of one water molecule maintains both conformations seen in the bare molecule. Here we present data for larger water clusters of TRA and IPA. This data provides evidence that the ability of water to form bridges between hydrogen bonding sites on the solute, can greatly influence the conformational preference of the parent molecule. Harmonic frequencies calculated by Density Functional Theory are compared to the infrared spectra to determine the structures of the water clusters. In the case of TRA-W_2 and TRA-W_3, water tends to form bridges between hydrogen binding sites of the molecule. The lowest energy structures of the solute molecule in the water clusters corresponds to the high energy structures in the bare molecule. Alternatively, in addition to maintaining the two conformations found in the bare molecule, the formation of the water dimmer bridge in IPA-W_2 produces two new conformations not found in the population of the monomer.