IR-IR PREDISSOCIATION SPECTROSCOPY OF PROTONATED TRIALANINE: BEGINNING TO DETERMINE HOW SIDE CHAINS AFFECT STRUCTURE AND SOLVATION

SUMMER LEE SHERMAN, KAITLYN C FISCHER, JONATHAN VOSS, ETIENNE GARAND, *Department of Chemistry, University of Wisconsin–Madison, Madison, WI, USA*.

Proteins and peptides are of interest to many different research groups across all fields of chemistry and biology. Of special interest is understanding conformational changes within proteins that occur due to different amino acid substituents, especially those that differ by just a side chain. However, it is very difficult to completely analyze a protein's full local environment due to spectral congestion from the different conformers of each protein. Thus, small peptides (N-chain, N=1-5) are used as model systems for both floppy and non-floppy chain systems to probe the effect of the R-group on the conformation population. Prior in the Garand group, conformations of protonated triglycine (Gly_3H^+) have been found for the bare peptide as well as when the peptide has one water molecule clustered around it. Therefore, in order to investigate how varying the side chain affects the conformations of these chained peptides, protonated trialanine (Ala_3H^+) is used due to the fact that the side chain here is changed from a hydrogen to a methyl group. Utilizing Cryogenic Ion Vibrational Spectroscopy (CIVS) and electronic structure calculations, highly resolved structural features of these systems will be elucidated. Conformer-specific IR-IR double resonance techniques will be used in to quantify the contribution of various conformers. This technique will allow the probing of how non-covalent interactions, with particular focus on intramolecular peptide H-bonding, change as a function of side chain. From these model systems, it will then be possible to extrapolate such characterization to larger peptides. Further on, through the use of microsolvation, it will be possible to determine the changes in conformation as a function of not only the side chain, but also through water-peptide H-bonding interactions.