CONFORMATION-SPECIFIC IR AND UV SPECTROSCOPY OF A MODEL SYNTHETIC FOLDAMER: β^3-ALA TRIPEPTIDE

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With the development of designed foldamers that that display biological activity and aid in drug delivery processes, there is an increasing interest in exploring the inherent conformational properties of model foldamers to understand better the subtle counter-balance of forces at play. β-amino acids have one additional backbone carbon atom that extends the spacing between amide groups, thereby providing a flexibility of construction, leading to secondary structures that either mimic or are complementary to those found in nature. Here we explore the secondary structures of foldamers in which the position of substitution of the methyl side chains of the Ala residues are switched from the β^2 to the β^3 position. In particular, we present data on a β^3-Ala tripeptide, Ac- β^3-Ala- β^3-Ala-β^3-Ala-NHBn under jet-cooled, isolated conditions. This talk will present conformation-specific IR and UV spectra using the techniques of resonant ion-dip infrared (RIDIR) spectroscopy and IR-UV holeburning, respectively. Following an exhaustive computational search of the conformational potential energy surface, low-lying minima are optimized and IR spectra calculated for comparison with the experimental RIDIR spectra. A single conformer is observed experimentally and assigned to a conformer with a C12/C8 hydrogen-bonded architecture that incorporates a 12-membered turn that is the β-peptide analog of a β-turn.