

SINGLE-CONFORMATION IR AND UV SPECTROSCOPY OF A PROTOTYPICAL HETEROGENEOUS α/β -PEPTIDE: IS IT A MIXED-HELIX FORMER?

KARL N. BLODGETT, PATRICK S. WALSH, TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN, USA.*

Synthetic foldamers are non-natural polymers designed to fold into unique secondary structures that either mimic nature's preferred secondary structures, or expand their possibilities. Among the most studied synthetic foldamers are β -peptides, which lengthen the distance between amide groups from the single substituted carbon spacer in α -peptides by one additional carbon. We present data on a mixed α/β tri-peptide in which a single β -residue with a conformationally constrained *cis*-2-aminocyclohexanecarboxylic acid (*cis*-ACHC) substitution is inserted in an α -peptide backbone to form Ac-Ala- β -ACHC-Ala-NHBn. This $\alpha\beta\alpha$ structure is known in longer sequences to prefer formation of a 9/11 mixed helix. Under isolated, jet cooled conditions, four unique conformers were observed in the expansion. The dominant conformer is configured in a tetramer cycle with every amide carbonyl and amine group involved in hydrogen bonding, giving rise to a tightly folded C12/C7/C8/C7 structure reminiscent of a β -turn. This talk will describe the conformation specific IR and UV spectroscopy methods used to study this mixed peptide, as well as its experimentally observed conformational preferences.