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Probing secondary structures of peptide chains using gas phase laser spectroscopy

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A bottom-up approach involving conformer-specific IR studies of short peptide sequences enables us to map the intramolecular interactions that shape the peptide backbone, in particular those H-bonds that are responsible for stability and formation of secondary structures in proteins, like turns or helices. The combination of laser-desorption of solid samples coupled to the efficient cooling in a supersonic expansion makes it possible to isolate in the gas phase the lowest conformations of the energy landscape of small flexible biomolecules. The low temperature achieved enables spectroscopists to record UV spectra in which the contribution of each conformer populated can be distinguished and the corresponding conformation identified using IR/UV double resonance spectroscopy. Data collected are directly comparable to the best quantum chemistry calculations on these species and therefore constitute a severe test for the theoretical methods used. It will be shown how investigation of sequences with an increasing number of building blocks permits to deduce the robust structural trends of a peptide backbone: i) local conformational preference of the backbone in one-residue chains, ii) in capped dipeptides, the competition between a succession of local conformational preferences and overall folded structures, in which a different type of H-bonding scheme, involving distant H-bonding sites along the backbone, takes place: in particular beta-turns, the secondary structure responsible for chain reversals, and finally iii) evidence for the spontaneous helical folding (short 3-10 helix) of three-residue chains will be presented, illustrating the relative weakness of the H-bonding in these molecular assemblies.