

# Experimental and computational approaches to determine conformational and stability principles of protein building units.

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## Abstract

Protein architectures show strong similarities regardless of the primary sequence of the molecule: the backbone folds of the different secondary structural elements exhibit rather similar geometrical properties even though composed of different amino acid residues. To decipher the principles of folding properties, a variety of oligopeptide models {e.g. HCO-(NH-L-CHR-CO)<sub>n</sub>-NH<sub>2</sub>} were amino acid residues have only a finite number of backbone studied. Natural folding types, all of different relative stabilities. The present lecture focuses on structure and stability issues of well known homo- and heteroconformers of peptides (such as  $\alpha$ -helix,  $\beta$ -pleated -turns sheet, collagen helix, *etc.*) optimized at *ab initio* levels of theory. The analysis of the relative energies associated with both *achiral* and *chiral* molecular conformers and supramolecular structures show how common secondary structure elements are gradually becoming more and more stable folds as the length of the polypeptide chain increases. The comprehensive analysis of over 200 fully optimized polypeptide structures reveals the same energy preference profile of major secondary structures as found in globular proteins.

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