H-bonding cooperativity and energetics of α-helix formation of five 17-amino acid peptides.

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Five peptides, each containing 17 amino acids, have been completely geometrically optimized in their α-helical and β-strand forms using a mixed DFT/AM1 procedure. B3LYP/D95** was used for the entire helical structures, while AM1 was initially used to optimize the side chains, followed by reoptimization at the DFT level. The energetic and structural results show (1) that the helices are favored over the strands by 29.5 to 37.4 kcal/mol; (2) that alkyl groups on the amino acid side chains favor helix formation even in the absence of solvent; (3) that C−H···O hydrogen bonds contribute to the relative stability of the helices that contain amino acids (val, leu and ile) with β-hydrogens in their alkyl side chains; (4) that formation of these helices entails approximately 6.6 kcal/mol of strain within the backbone per hydrogen bond; and (5) that H-bond cooperativity is essential for the α-helix to become more stable than a corresponding β-strand. This last observation strongly suggests that pairwise potentials are inadequate for modeling of peptides and proteins.

Słowa kluczowe

Alkyls, Chemical structure, Energy, Monomers, Peptides and proteins

Adres publiczny

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