MS-4

Conformational Role of Proline in α-Helices

Young Kee Kang and Mee Kyoung Kim*
Dept. of Chemistry, Chungbuk National University

Conformational energy calculations have been carried out for proline-containing alanine-based pentadecapeptides with the sequence Ac-$(Ala)_n$-Pro-$(Ala)_m$-NHMe (n + m = 14), in order to figure out the positional preference of proline in α-helices. The conformational energy was computed a sum of the potential energy (ECEPP/3) and the hydration free energy computed by the hydration shell model. The relative energy of each peptide was calculated by subtracting the energy of the all extended conformation from that of α-helical one, which is used here as a measure of preference. The highest preference is found for the peptide with proline at Ncap + 1 position, and the next preferences are found at Ncap, N'(Ncap - 1), and C'(Ccap + 1) positions. These computed results are consistent with the positional preferences estimated from X-ray structures of proteins. Close contacts between residues neighboring proline are found to play a role in destabilizing kinked α-helical conformations, which was expected from the analysis of protein structures. The favored electrostatic and nonbonded energies as well as the favored hydration of the imide nitrogen of proline appears to contribute significantly to the highest preference of proline at the beginning of α-helix.