

Self-organized Structures of Homooligopeptides of α - and β -Amino Acid Bearing Nonplanar Amide Bonds, and Functionalization of Helix Surfaces

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【Outline of survey】

The planarity of amide bonds intrinsically contributes to the construction of peptide secondary structures, helix and strand, which underlies restricted conformations of peptide units. Significant roles of the planarity of amide bonds in secondary structures have been suggested even in β -amino acid oligomers, as well as α -amino acid peptides. Bicyclic 7-azabicyclo[2.2.1]heptane amides take intrinsically nonplanar structures, i.e., they exhibit nitrogen-pyramidalization and twisting with respect to the N-C(=O) bond, in solid, solution, and gas (computation) phases. We designed chiral α - and β -amino acid derivatives of a 7-azabicyclo[2.2.1]heptane skeleton, synthesized several homooligomers, and examined whether self-organized structures occur in solution. In the present case of the tertiary amide, the absence of a hydrogen atom on the amide nitrogen rules out the formation of hydrogen bonding to carbonyl oxygen atoms.

【Expected results】

The present study will reveal whether or not planarity of amide bonds is relevant to the self-organized structures of peptides. In practical view point, we will show that homooligomers of bicyclic α - and β -amino acids with the 7-azabicyclo[2.2.1]heptane scaffold take self-organized structures, irrespective of the nonplanar amide bond and the absence of N-H...O=C internal hydrogen bonding. This result will have a great impact on the molecular mechanisms of protein (or peptide) folding process. For the application of this study, we can synthesize helix molecules, which can control the assembly of the helices, i.e., helix bundles, through the interaction of the functional groups on the helix surfaces.

【References by the principal researcher】

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【Homepage address】 <http://www.f.u-tokyo.ac.jp/~yakka/>