

环十二肽溶液构象的二维核磁共振研究

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摘要

利用二维核磁共振方法及距离几何计算研究了在片段组装法全新蛋白质合成中用作底座分子的环十二肽的溶液构象.

研究表明在环十二肽分子主链中包含四个转角结构,四个赖氨酸侧链均位于环的同一侧.

环肽的构象为以环肽为模板组装四螺旋束分子提供了有利的条件

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Studies on 2D-NMR of the solution conformation of a dodecacyclopeptide

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Abstract A dodecacyclopeptide, which was used as a supporting template in template assembled synthetic approach for four-helix-bundle proteins, was studied by solution 2D-NMR and distance geometry calcns. All hydrogen atoms in the mol. were assigned by anal. of its 2D-COSY and NOESY spectra. DIANA distance geometry calcns. were carried out with 62 interat. distances derived from NOE cross peak intensities. Among the 100 structures obtained, the top 10 structures with lowest target function values were selected as final results. The main chain atom r.m.s. between this 10 structures was 0.029 ?0.006nm, showing very rigid conformation of the dodecacyclopeptide mol. The four lysine side chains used as attaching points for four helix were found facing towards the same side of the cyclopeptide ring, showing the validity of utilizing this dodecacyclopeptide in the synthesis of four-helix-bundle proteins.

Key words

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