化学学报 1996 54 (7): 702-708 ISSN: 0567-7351 CN: 31-1320/06

寡肽**Asterin B**和**C**溶液构象的**NMR**研究 Ⅱ**. NMR**及分子动力学模拟

高金海,石根斌,宋国强,陈凯先,嵇汝运

中国科学院上海药物研究所

收稿日期 修回日期 网络版发布日期 接受日期

摘要 利用NMR和分子动力学方法研究了寡肽Asterin B和C的溶液构象。结果表明,Asterin B在溶液中形成了某种非氢键的转角结构, 并由残基间的疏水相互作用使整个分子具有两亲性, 这种结构特征可能和其生物活性有关。并进一步讨论了这种结构的形成在蛋白质卷曲的起始过程中的意义。而Asterin C在溶液中柔性较大, 存在多种构象的平均。

关键词 寡肽 分子动力学 疏水作用 溶液构象 二维核磁共振

分类号 R91

Conformational studies of Asterin B and C in solution by NMR Ⅱ. Conformational analysis by NMR and molecular dynamic simulations

GAO JINHAI,SHI GENBIN,SONG GUOQIANG,CHEN KAIXIAN,JI RUYUN

Abstract The conformational properties of two pentapeptides Asterin B (△ Pro-Thr-Ser-βPhe-Abu-OMe, 1) and Asterin C (△Pro-Abu-Ser-βPhe- Thr-OMe, 2), isolated from Chinese traditional medicine Aster tataricus, have been investigated by 2D-NMR and restrained molecular dynamic calculations (RMD). The solution conformation of 1 was characterized as a nonclassic β-turnstructure at (△Pro-Thr-Ser-β Phe) region with an amphiphilic feature, which may be related to its antitumor activity against P388 leukemia. There is no evidence in the form of lowered amide proton temperature coefficients for direct hydrogen bonding as a primary source of turn stability. Instead, the major stabilization appears to be the hydrophobic interaction between aromatic rings (△Pro and βPhe). Implications for stabilization of this unusual turn structure during the earliest events in protein folding are discussed. The conformation of 2 in solution was shown to be more flexible with multiple conformational averaging.

Key words OLIGOPEPTIDE MOLECULAR DYNAMICS

DOI:

通讯作者