#### 寡肽Asterin B和C溶液构象的NMR研究1: ^1H NMR归属及构象特征

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摘要 Asterin B和C是从紫菀中分得的两个寡肽,本文利用2D-NMR技术归属了它们的^1H NMR谱线,并讨论了它们的构象特征。为进一步采用NMR和分子动力学(MD)方法研究它们的溶液构象奠定了基础。关键词 <u>寡肽 质子磁共振谱法 紫菀 分子动力学 溶液构象 二维核磁共振</u>

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### Conformational studies of asterin B and C in solution by NMR

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Abstract Several 2D NMR techniques have been used to assign all proton resonances of Asterin B and C, which were biologically active peptides isolated from Aster tataricus. Recognition of the amino acid spin systems has been achieved by COSY spectra, including two new residues ( $\Delta$ Pro and  $\beta$ Phe) in plant peptide. The sequential assignments were obtained based on the combination of COSY and NOESY spectra and confirmed the amino acid sequence in both peptides. These assignments provide an essential foundation for elucidation of their solution conformations based on NMR data and restrained MD simulations.

**Key words** OLIGOPEPTIDE PROTON MAGNETIC RESONANCE SPECTROMETRY ASTER TATARICUS MOLECULAR DYNAMICS

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