马氏钳蝎短链神经毒素BmP03的溶液结构的NMR研究

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摘要 BmP03为从马氏钳蝎中得到的具有钾离子通道阻断活性的短链神经毒素。应用 2DNMR实验和分子模拟技术,进行BmP03的溶液结构计算,结果显示BmP03 与从蝎毒中得到的其他短链神经毒素具有相似结构。含一个α-螺旋(Cys3-Gly12),两条反平行的β-折叠股(Asn16-Cys19,Cys24-Asn27)。螺旋与折叠股间靠3对二硫键相连,在Asp20到Val23

间形成一个二型转角结构。根据BmP03的溶液结构,对其表面电荷对钾离子通道阻断活性的影响进行观察。 关键词 <u>马氏钳蝎</u> <u>神经毒素 溶液结构 二维核磁共振</u>

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Three-dimensional structure of BmP03 from venom of scorpion buthus martensii karsch

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Abstract From the venom of scorpion Buthus martensii Karsch, a short peptide (BmP03, 28 amino acid residues) was isolated, characterized and tested as a weak inhibitor of K^+ channel. In this paper, the solution structure of BmP03 was determined by 2D ^1H NMR spectroscopy and molecular modeling calculations. The conformation of BmP03 is composed of a short α -helix (Cys3-Gly12) and a two-strand antiparallel β -sheet (Asn16-Cys19, Cys24-Asn27). There are three disulfide bridges (Cys3-Cys19, Cys6-Cys24, Cys10-cys26) connecting the α -helix and β -sheet. Asp20 to Val23 residues form a type II turn linking the two strands. Structural and electrostatic potential comparison between BmP03 and its analogues were also presented.

Key words <u>NEUROTOXINS</u>

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