

胃泌素有关肽溶液构象的2D-NMR研究

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摘要 用2D NMR深入研究了五肽、四肽胃泌素在 DMSO 中的构象。利用 COSY 谱、Relayed-COSY 谱、DQF-J 分解谱和 NOESY 谱归属了全部共振峰。计算了肽键平面的 Φ 角、旋转异构体分布和旋转异构体之间自由能差。根据 NOESY 谱得到了距离约束条件。结合 Φ 角及旋转异构体分布,推导出五肽胃泌素分子的构象膜型。结果表明,五肽、四肽胃泌素在 DMSO 中以半角构象存在,在其主要的旋转异构体中 Trp 的吲哚环和 Met 的 S 原子具有类似 5,1-benzothiazocine 三维结构,可能是具有生物活性的原因。

关键词 [寡肽](#) [构象](#) [热带林](#) [二维核磁共振谱法](#) [四肽](#) [胃泌素](#) [五肽](#) [溶液构象](#) [DMSO](#) [COSY谱](#) [DQF-J分解谱](#) [NOESY谱](#)

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The study of conformations in solution for gastrin with 2D NMR

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Abstract Conformations of Boc-pentapeptide (Boc-b-Ala-Trp-Met-Asp-PheNH₂) and Boc-tetrapeptide (Boc-Trp-Met-Asp-PheNH₂) of gastrin in DMSO solns. were investigated by 2-dimensional (2D) NMR spectrometry. 2D COSY, Relayed-COSY, DQF-J Resolved Spectroscopy and NOESY were applied to assign all resonance lines completely, F dihedral angles, rotamer populations, and their energy differences were calculated According to NOE, conditions of distance constraints were obtained. Taken together with F and rotamer populations, the model of conformation for Boc-pentapeptide was obtained. Conformations of Boc-pentapeptide and Boc-tetrapeptide are characterized by half turn in DMSO solution In their main rotamers, indole of Trp and S atom of Met form a 3-dimensional structure similar to 5,1-benzothiazocine, and this structure may be the cause of biol. potency.

Key words [OLIGOPEPTIDE](#) [CONFORMATION](#) [TROPICAL FOREST](#) [2D NMR SPECTROMETRY](#) [GASTRIN](#) [PENTAPEPTIDE](#)

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