

论文

盐酸西替利嗪的NMR研究

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摘要:

目的研究盐酸西替利嗪在DMSO-d₆溶剂中的核磁共振现象并对其质子和碳信号进行归属。方法测定其在不同温度和加入重水条件下的各种1D和2D核磁共振谱。结果室温下以DMSO-d₆为溶剂时, 哌嗪环及与其N原子相连的碳、氢信号均呈现多个峰或宽峰, 提高温度或加入重水后, 其碳、氢信号均出现“合并”或变窄现象。结论室温下在DMSO-d₆溶剂中, 与核磁共振“时间尺度”相比, 不同构象的盐酸西替利嗪并存; 随着温度的提高, 不同构象能快速互变, 而加入重水则形成稳定构象。

关键词: 盐酸西替利嗪 核磁共振 变温试验 构象分析

NMR studies on cetirizine hydrochloride

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Abstract:

Aim To study the NMR phenomena of cetirizine hydrochloride and assign all proton and carbon signals in NMR spectra. Methods To record the 1D and 2D NMR spectra of cetirizine hydrochloride while changing the experimental temperature and adding D₂O into the solution. Results More than one NMR signal or broad peak resulting from piperazine and the attached groups with N atom were given in DMSO-d₆ solution at room temperature. "Coalescence" or narrowing had occurred for the proton and carbon signals when the experimental temperature was increased or D₂O was added into the solution. Conclusion Compared with the NMR "time scale", there are more than one conformation of cetirizine hydrochloride in DMSO-d₆ solution at room temperature. The different conformation will be exchanged fast while temperature rised and the stable conformation will be existed while D₂O was added into the solution.

Keywords: NMR varied temperature experiment conformation analysis cetirizine hydrochloride

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