

论文  
用NOE差谱和二维核磁共振技术研究3S-取代烷氧基-奎宁环烷的立体化学

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摘要:

用3S-奎宁环醇与环氧化合物反应,得到化合物(I)的二个光学异构体(3S-1)和(3S-2)。它们的生物活性有明显差别。本文采用NOE差谱和二维NMR技术指定了各异构体的绝对构型。用<sup>1</sup>H和<sup>13</sup>C信号的归属,确定了它们的溶液态构象,测定了其C-11的绝对构型。测定结果经X-射线衍射测定进一步得以肯定。

关键词: 二维核磁共振 NOE差谱 抗胆碱物 非对映异构体 绝对构型

<sup>1</sup>H, <sup>13</sup>C NMR AND STEREOCHEMISTRY STUDIES OF 3SSUBSTITUTED ALKOXYLQUINUCLIDINE BY TWO-DIMENSIONAL AND NOE DIFFERENCE NMR TECHNIQUES

ZC Miao; JH Gao; R Feng and OK Zhang

Abstract:

By using optically pure 3S-quinuclidinol, two diastereoisomers(3S-1) and (3S-2) of 3-(substituted) alkoxy-quinuclidine were synthesized. <sup>1</sup>H and <sup>13</sup>C NMR spectra of (3S-1) and (3S-2) have been completely analyzed utilizing doublequantum filtered COSY, <sup>13</sup>C-<sup>1</sup>H COSY and NOE difference experiment. The NOE difference experiment was used to determine the absolute configuration at C-11 of the diastereomers. According to the results of NOE difference and variable concentration NMR experiments, the configuration about C-11 of (3S-1) is designated as R (1A), whereas the configuration about C-11 of (3S-2) is designated as S (1B). The result was confirmed by X-ray diffraction analysis.

Keywords: NOE Difference experiment Anticholinergics Diastereomer Absolute configuration Two-dimensional NMR

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