

论文

固相萃取—核磁氢谱法研究曲美布汀的代谢产物

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摘要:

目的:用固相萃取—核磁共振谱法探索曲美布汀在体内的代谢产物。方法:用固相萃取柱将大鼠尿液的内源性物质从样品中去除,然后进行连续样品¹HNMR谱的测定,经结构片段的解析,将其峰积分进行匹配,推断可能的代谢产物,并指出未发生代谢的部位。结果:曲美布汀酯水解产物在代谢产物中是主要成分,其中醇部分的进一步代谢是主要的代谢途径。与文献报道的同位素方法研究结果相同。结论:代谢产物混合物的¹HNMR谱可经结构片段解析和峰积分匹配来推测代谢产物,此法简便,提供的信息可帮助了解药物在体内的转化。

关键词: 固相萃取 核磁共振谱 曲美布汀 药物代谢

STUDY ON METABOLITES OF TRIMEBUTINE WITH SOLID PHASE EXTRACTION (SPE) —¹HNMR COMBINATION

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Abstract:

AIM: In order to assess the applicability of combined usage of solid phase extraction (SPE) and nuclear magnetic resonance spectroscopy (NMR) in the study of metabolites, trimebutine was selected, which is a compound composed of two parts by ester linkage. METHODS: With SPE the endogenic compounds were removed efficiently, and ¹HNMR was performed for the eluates. After resolving the structure of each piece, the metabolites were predicted, and the non-metabolized positions were pointed out. RESULTS: The hydrolyzed products were the main metabolites of trimebutine, and the main pathway of the metabolism occurred in the part of butanol. The results agree with those by using isotopic method reported in the literature. CONCLUSION: The experiment showed that if the structures of the pieces were confirmed, and they were fitted together with the matching principle of the peak area integral in one compound, the metabolites could be predicted. This method can provide information of the metabolism and it is convenient in operation.

Keywords: nuclear magnetic resonance spectrum trimebutine drug metabolism solid phase extraction

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