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论文

LC/MS分析大鼠体内氧化苦参碱及其主要代谢物LC/MS分析大鼠体内氧化苦参碱及其主要代谢物

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摘要：

目的研究氧化苦参碱在大鼠体内的主要代谢产物。方法以氧化苦参碱和苦参碱为对象优化液相色谱/电喷雾离子阱质谱(LC/ESI-ITMS^n)实验条件，分析总结其电喷雾质谱的一级电离规律和二级质谱裂解规律，作为氧化苦参碱大鼠体内代谢物结构分析的依据。健康大鼠腹腔肌注40 mg·kg^{-1}氧化苦参碱，收集0~24 h的尿样，尿样中的代谢物经C_{18}小柱进行富集与纯化后，在优化的LC/ESI-ITMS^{n}条件下进样分析。代谢物的结构推导主要依据代谢物的色谱保留时间及其电喷雾离子阱质谱(ESI-ITMS^n)电离规律。结果在大鼠尿样中有原药及其6种I相氧化及还原代谢产物，且主要代谢物为苦参碱。未发现II相代谢物。结论本法不仅操作简便、快速，而且灵敏度高、专属性强。该分析技术是研究药物代谢最有效的方法之一。

关键词： LC/ESI-ITMS^n 氧化苦参碱 代谢物

HPLC-electrospray ionization ion trap tandem mass spectrometry analysis of oxymatrine and its metabolites in rat urine

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Abstract:

AimTo identify the main metabolites of oxymatrine (OMT) in rats. MethodsTo optimize the conditions of LC/ESI-ITMS^n chromatograms and spectra by oxymatrine and matrine (MT), and summarize their ionization and cleavage rules in ESIMS, then serving as the basis for the metabolite analyses of oxymatrine in rats. To collect the 0-24 h urine samples of the rats after ip 40 mg·kg^{-1} oxymatrine, the samples were enriched and purified through C_{18} solid-phase extraction cartridge. The purified samples were analyzed by LC/ESI-ITMS. The structures of OMT metabolites were identified according to their retention times and ESI-ITMS^n rules. ResultsSix phase I metabolites and the parent drug OMT were found in the rat urine, and the main metabolite was MT. No phase II metabolites were found. ConclusionThe developed LC/ESI-ITMS^n methods to identify the metabolites of oxymatrine in rats is not only simple and rapid but also sensitive and specific. This technology is one of the most efficient methods for the analysis of drug metabolites.

Keywords: oxymatrine metabolite LC/ESI-ITMS^n

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