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论文

LC-MS/MS法研究1- [1-(6-甲氧基-2-萘基)乙基]-2-(4-硝基苄基)-6,7-二甲氧基-1,2,3,4-四氢异喹啉氢溴酸盐在大鼠体内的代谢产物

王雷娜;宋敏;杭太俊;张正行

中国药科大学 药物分析教研室, 江苏 南京 210009

摘要:

采用液相色谱-串联质谱法对大鼠灌胃1- [1-(6-甲氧基-2-萘基)乙基]-2-(4-硝基苄基)-6,7-二甲氧基-1,2,3,4-四 氢异喹啉氢溴酸盐(编号P91024)后粪便、尿液、胆汁和血浆中的主要代谢产物进行研究。通过比较给药样品和空 白样品的全扫描总离子流色谱和选择离子扫描色谱图差别寻找1相代谢产物:根据其一级和二级质谱图,确定1相代 谢产物的分子结构。完全提取Ⅰ相代谢产物后的样品溶液,再用葡糖醛酸酶酶解,得Ⅱ相结合物的苷元部分,采用 与Ⅰ相代谢产物鉴定同样方法寻找和鉴定Ⅱ相代谢产物苷元的结构,进而确证Ⅱ相代谢产物的分子结构。从大鼠粪便 中鉴定出P91024的2个I相代谢物,从胆汁中鉴定出1个I相和5个II相代谢产物,从尿液中鉴定出1个I相和3个II相 代谢产物,从血浆中鉴定出4个I相和1个II相代谢产物;并分别分析推测出它们的结构。P91024在大鼠体内被代谢 转化为多种产物,利用LC-MS/MS可以快速寻找和鉴定。

关键词: 1- [1-(6-甲氧基-2-萘基)乙基]-2-(4-硝基苄基)-6,7-二甲氧基-1,2,3,4-四氢异喹啉氢溴酸盐 代谢 物 液相色谱-串联质谱

Metabolites of 1-(1-(6-methoxyl-2-naphthyl)ethyl)-2-(4-nitrobenzyl)-6,7dimethoxyl-1,2,3,4-tetrahydroisoquinoline hydrobromide in rat by LC-MS/MS method

WANG Lei-na; SONG Min; HANG Tai-jun; ZHANG Zheng-xing

Abstract:

To investigate the principal metabolites of 1-(1-(6-methoxyl-2-naphthyl)ethyl)-2-(4-nitrobenzyl)-6,7dimethoxyl-1,2,3,4-tetrahydroisoquinoline hydrobromide (code designation: P91024) in rats after ig administration by LC-MS/MS, the phase I metabolites were discovered by comparing the fullscan and SIM chromatograms of the test samples with the corresponding blanks. The structures of phase I metabolites were identified by ESI-MS spectra and the product spectra of the corresponding adduct ions. The phase II metabolites were identified in the test samples after the phase I metabolites were completely removed with solvent extraction and then treated with glucuronidase for enzymolysis of phase II glucuronide conjugates and the hydrolysates. Two phase I metabolites of P91024 were identified in rat feces, one phase I and five phase II in bile, one phase I and three phase II in urine, and Article by four phase I and one phase II in plasma. Their structures were elucidated, separately. P91024 was extensively metabolized in rat. The metabolites can be easily screened and identified by LC-MS/MS method.

Keywords: metabolite LC-MS/MS 1-(1-(6-methoxyl-2-naphthyl)-2-(4-nitrobenzyl)-6,7dimethoxyl-1,2,3,4-tetrahydroisoquinoline hydrobromide

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作者简介:

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- ▶代谢物
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