

论文

电喷雾离子阱质谱法直接测定几种药物的葡萄糖苷酸型代谢物

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摘要:

为研究药物代谢产物的质谱规律,用电喷雾离子阱质谱法对溶液中乙氧苯柳胺、SFZ-47羧基衍生物、5-羟基普罗帕酮及普罗帕酮的 β -D-葡萄糖苷酸型代谢物的结构进行了测定。结果表明,它们的(-)ESI-MS均生成[M-H]⁻准分子离子,(-)ESI-MS²和(-)ESI-MS³则分别生成m/z175和m/z113碎片离子。提示这些共同特征可用于LC/MS法直接分析药物的葡萄糖苷酸型代谢物。

关键词: 电喷雾离子阱质谱法 代谢物 葡萄糖苷酸

CHARACTERIZATION OF SOME GLUCURONIDE CONJUGATES BY ELECTROSPRAY ION TRAP MASS SPECTROMETRY

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Abstract:

To investigate the characteristics of mass spectra of some drug metabolites, solutions of glucuronide conjugates of *N*-(4-ethoxyphenyl)-2-hydroxyl-benzamide (etofesalamide), 4-(3H-1,2-dihydro-1-pyrrolizinone-2-methylamino)-benzoic acid, 5-hydroxypropafenone and propafenone were analyzed using electrospray ion trap mass spectrometry in a multi-stage full scan mode performed on a Finnigan LCQ instrument. Sample solutions were directly introduced into the ESI source at a flow rate of 15~30 μ l·min⁻¹ by a syringe pump. The mass spectrometer was operated in the negative ion mode. A full scan mass spectra of each analyte provided quasimolecular ion m/z M-1⁻, and full scan MS² and MS³ spectra gave characteristic fragment ions m/z 175 and m/z 113, respectively, which were derived from the glucuronate moiety of each analyte. The proposed interpretation of m/z 175 is the negative ion of glucuronic acid with a loss of 18 u (H₂O), which produces m/z 113 after further losing 18 u (H₂O) and 44 u (CO₂). Fragmentation pathway has been established for each analyte. The results show that quasimolecular ion m/z M-1 and the characteristic fragment ions m/z 175 and m/z 113 in the multi-stage full scan mass analysis of each analyte can be predicted for future structure elucidation or quantitative determination of glucuronide conjugates by LC/MS.

Keywords: Drug metabolites Glucuronide conjugates Electrospray ion trap mass spectrometry

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