

论文

中国红豆杉细胞培养物中紫杉烷的LC-ESI-MS代谢轮廓分析  
中国红豆杉细胞培养物中紫杉烷的LC-ESI-MS代谢轮廓分析

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摘要:

目的建立小剂量生物样中紫杉烷的快速分析方法,为紫杉烷代谢特征研究提供新的分析方法和手段。方法用LC-ESI-MS方法,先对包含了5种已知成分的紫杉烷混合溶液进行分析,以调整和优化质谱运行参数。随后正离子和负离子方式同时扫描,获得样品的总离子流图和多个色谱峰的相对分子质量信息,通过选择离子监控(SIM)对准分子离子峰进行MS/MS测定,分析化合物的结构特点和主要取代基,结合文献检索和遗传相关性分析,推测紫杉烷的结构。结果毛细管电压为25 V、碰撞诱导能量为25 eV时,获得较好的一级和二级质谱信号。具有多个乙酰取代基的紫杉烷在正离子扫描时,产生强的铵加合离子峰,含多个羟基的紫杉烷易产生质子加合峰。对样品中13个色谱峰进行了指认,其中8个经对照品和文献的比较可以确定其分子结构,另外5种可以推测紫杉烷母核的类型和取代基的数目和种类。结论用LC-MS方法快速分析样品中紫杉烷的类型及其变化是可行的,为研究紫杉烷的代谢规律提供了有力的分析工具。

关键词: 红豆杉 细胞培养物 紫杉烷 代谢轮廓分析 LC-MS ESI-MS/MS

LC-ESI-MS metabolic profiling analysis of taxanes from the extracts of *Taxus chinensis* cell cultures

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Abstract:

Aim To develop a rapid analytical method for small amount biological samples of taxanes by using liquid chromatography coupled with electrospray ionization tandem mass spectrometry (LC-ESI-MS) in small amount biological samples. Methods A solution containing five given taxane constituents and the extract from cell cultures of *Taxus chinensis* were analysed separately. According to the performance of the given taxanes in ESI-MS/MS, run parameters of the mass spectrometer were optimized. Positive and negative electrospray modes were employed to simultaneously scan the cell cultures sample, and the full ion chromatogram and the molecular weight of individual peak were obtained. The qualitative analysis of taxanes was achieved by comparison of the retention time and molecular weight with those of the reference substances or was based on the interpretation of the MS/MS spectra of the analytes and the knowledge of the concerning genetic backgrounds of taxanes published in literatures. Results The taxanes with several acetyl substituents tended to produce ammonium adduct ions peak, while multi-hydroxy taxanes were subject to give protonized molecular ion peaks in positive ion ESI-MS. Thirteen taxanes in cell samples were assigned. Eight compounds of them were identified to be 1-acetyl-5,7,10-deacetyl-baccatin I (DAB-I, 1), baccatin III (B-III, 3), baccatin VI (B-VI, 8), taxol (9), yunnanxane (10), taxuyunnanine C (Tc, 11), sinenxane B (12), sinenxane C (13), separately. For the other five constituents, character of taxane and the number of substituents were deduced. Conclusion The results confirm the feasibility of characterizing taxanes in biological samples by LC-ESI-MS analysis. The analytical methodology provided a rapid, conventional and reliable tool to study metabolic profiling of taxanes for structural elucidation in taxol biosynthesis.

Keywords: cell culture taxanes metabolic profiling analysis LC-MS ESI-MS/MS *Taxus chinensis*

收稿日期 2004-09-15 修回日期 网络版发布日期

DOI:

基金项目:

通讯作者: 余龙江

作者简介:

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