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研究论文

高效液相色谱/电喷雾-离子阱-飞行时间质谱分析鉴定中药虎杖中的主要化学成分

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摘要 建立了快速、准确鉴别中药虎杖中化学成分的液相色谱-质谱法。采用高效液相色谱/电喷雾-离子阱-飞行时间质谱(HPLC/ESI-IT-TOF MS)对蒽醌类以及羟基二苯乙烯类对照品, 包括大黄素、大黄酚、大黄素甲醚、大黄酸、芦荟大黄素和虎杖苷进行了分析, 总结其多级裂解规律。建立了虎杖甲醇提取物的液相色谱分离条件及质谱检测条件, 根据负离子模式下获得的各组分多级质谱数据, 对比对照品碎裂特征并参考文献, 对主要色谱峰进行指认, 共鉴别了10个化合物, 包括白藜芦醇-4′-O-葡萄糖苷、虎杖苷、大黄素-8-O-葡萄糖苷、白藜芦醇、决明松-8-O-葡萄糖苷、大黄素-1-O-葡萄糖苷、决明松-8-O-(6′-乙酰基)葡萄糖苷、大黄素甲醚-8-O-葡萄糖苷、大黄素甲醚-8-O-(6′-乙酰基)葡萄糖苷和大黄素, 其中决明松-8-O-(6′-乙酰基)葡萄糖苷和大黄素甲醚-8-O-(6′-乙酰基)葡萄糖苷为虎杖中新发现的成分。研究结果表明, 在中药化学成分研究工作中, 采用电喷雾-离子阱-飞行时间质谱可提高中药化学成分的分析效率并有利于新化合物的发现和鉴别。

关键词 高效液相色谱 电喷雾-离子阱-飞行时间质谱 主要成分 鉴定 虎杖 中草药

Identification and determination of major constituents in Polygonum cuspidatum Sieb. et Zucc. by high performance liquid chromatography/electrospray ionization-ion trap-time-of-flight mass spectrometry

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Abstract

A facile method using high performance liquid chromatography/electrospray ionization-ion trap-time-of-flight mass spectrometry (HPLC/ESI-IT-TOF MS) has been established for the analysis of multiple constituents in Polygonum cuspidatum Sieb. et Zucc. Six chemical standards including emodin, chrysophanol, physcion, rhein, aloe-emodin and polydatin were studied systematically and their fragmentation pathways were concluded. The methanol extract of Polygonum cuspidatum Sieb. et Zucc. was separated and analyzed by HPLC/ESI-QIT-TOF MS system in negative ion mode. A total of 10 constituents were identified or tentatively characterized with supporting results on the fragmentation pathways of 6 chemical standards and relative references. These constituents are mainly anthraquinones, stilbenes, torachryson and their derivatives, including resveratroloside, polydatin, emodin-8-O-glucoside, resveratrol, torachryson-8-O-glucoside, emodin-1-O-glucoside, torachryson-8-O-(6′-acetyl)glucoside (newly discovered), physcion-8-O-glucoside, physcion-8-O-(6′-acetyl)glucoside (newly discovered) and emodin. It is an extremely simple way by using HPLC/ESI-IT-TOF MS to provide chemical information concerning the constituents in herbal medicines and making the identification results more convinced.

Key words high performance liquid chromatography (HPLC) electrospray ionization-ion trap-time-of-flight mass spectrometry (ESI-IT-TOF MS) major constituent identification Polygonum cuspidatum Sieb. et Zucc. Chinese herbal medicine

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