

全二维气相色谱/飞行时间质谱分析不同产地的川芎挥发油

王楠¹, 张艺^{2*}, 李响¹, 童应鹏², 孔宏伟^{1*}, 许国旺^{1*}

1. 中国科学院大连化学物理研究所, 中国科学院分离分析重点实验室, 辽宁 大连 116023; 2. 成都中医药大学, 四川 成都 61003

Analysis of volatile oils of *Ligusticum chuanxiong* Hort. from c origins by comprehensive two-dimensional gas chromatograp spectrometry

WANG Nan¹, ZHANG Yi^{2*}, LI Xiang¹, TONG Yingpeng², KONG Hongwei^{1*}, XU Guowang^{1*}

1. Dalian Institute of Chemical Physics, Key Laboratory of Separation Science for Analytical Chemistry, Chinese
2. Chengdu University of Traditional Chinese Medicine, Chengdu 610031, China

摘要

参考文献

相关文章

Download: PDF (400KB) [HTML](#) 0KB Export: BibTeX or EndNote (RIS) Supporting Info

摘要 建立了川芎挥发油的全二维气相色谱/飞行时间质谱(GC×GC/TOF MS)指纹图谱,并结合聚类分析评价了川芎药材的质量。4种类物质在DB-Petro×DB-17柱系统上实现了明显的族组分分离。从新都市的1个样品中分离出375种组分,其中相似度、反相似度皆化合物215个;根据质谱库检索和保留指数验证,或参照标准化合物及文献报道,从中定性了43个化合物。结合偏小二乘法-判别分析将4个产区的挥发油样品加以区分,并找出20种差异最大的化合物,其中包括4种苯酐类物质。在此基础上,进一步应用正交偏小二乘成分和抗氧化活性,结果发现,苯酐类物质(如藜本内酯、川芎内酯A和新蛇床内酯)对川芎挥发油样品地区差异的影响最大,其中彭州产酐类物质的含量最高。本文通过高分辨色谱技术研究了相邻产地的药物化学组成差异,并将化学指纹及生物学活性相关联,建立了系统评价及活性化合物筛选研究模式。

关键词: 全二维气相色谱/飞行时间质谱 挥发油 苯酐 质量控制 川芎

Abstract: The volatile oils of 23 *Ligusticum chuanxiong* Hort. samples from 4 different regions were analyzed comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry (GC×GC/TOF MS). The separation of 4 terpenoids and phthalides was well accomplished based on a DB-Petro×DB-17 column system. MS library search, 215 compounds were tentatively identified based on the NIST database and the 43 compounds were confirmed by using the retention index or comparing with the standard compounds in a typical sample from Xindu City. Twenty three samples were apparently classified into 4 groups by partial least square-discriminant analysis. A brief list of 20 differential compounds is presented, including cnidilide, 3-n-butylphthalide and butylidene phthalide. DPPH (1,1-diphenyl-2-picrylhydrazyl) stable free radical scavenging assay was adopted to differentiate the antioxidant activity of these samples, which was expressed as EC₅₀. Based on the orthogonal partial least square mode biochemical discrimination of samples was achieved with ligustilide, senkyunolide A and neocnidilide as important differential compounds according to geographical origins. All the results indicated that phthalides exert a great influence on the chemical and biochemical classifications of *Rhizoma Chuanxiong*, and the samples from Pengzhou City had the highest contents of phthalides.

Keywords: comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry (GC×GC/TOF MS) volatile oil phthalide quality control *Ligusticum chuanxiong* Hort.

Received 2009-12-28; published 2010-04-28

Corresponding Authors: 孔宏伟, 张 艺

引用本文: