

基于非靶向代谢组学和生物信息学的参芪肾衰合剂抗肾纤维化质量标志物的筛选与定量分析^Δ

周宇航^{1,2*}, 李玉琪^{1,2}, 高 苗^{1,2}, 阮清锋², 曾晓璇², 王 慧³, 黄传奇^{1,2}, 徐宏峰^{1,2#}[1. 湖北中医药大学药学院, 武汉 430065; 2. 武汉市第一医院药学部, 武汉 430022; 3. 湖北省药品(医疗器械)不良反应监测中心, 武汉 430060]

中图分类号 R917 文献标志码 A 文章编号 1001-0408(2026)13-1716-06
DOI 10.6039/j.issn.1001-0408.2026.13.10



摘要 **目的** 筛选并定量分析参芪肾衰合剂(SQSS)中与抗肾纤维化相关的质量标志物(Q-Marker),为SQSS的药效物质分析和新药转化提供参考。**方法** 采用非靶向代谢组学技术对SQSS化学成分进行解析;整合网络药理学、基因表达综合数据库、连接图谱数据库等,筛选SQSS抗肾纤维化的Q-Marker。采用高效液相色谱-串联质谱法定量分析10批SQSS中Q-Marker的含量。**结果** 基于非靶向代谢组学技术从SQSS中共鉴定出1 319种化合物,进一步筛选出具有抗肾纤维化作用的活性成分84个(如芒果花素等)。基于网络药理学、基因表达综合数据库等共筛选出9个抗肾纤维化Q-Marker(分别为小檗碱、槲皮素、和厚朴酚、烟酰胺、大豆苷元、香豆素、山柰酚、芒果花素、苦杏仁苷)。定量分析结果显示,10批SQSS中上述成分(苦杏仁苷除外)的平均含量分别为2.523、1.942、26.848、1.415、0.692、0.171、0.374、7.401 μg/mL。**结论** 本研究筛选出SQSS抗肾纤维化的9个Q-Marker,并对其8个成分进行了含量测定,可为SQSS的药效物质基础解析和新药转化提供参考。

关键词 参芪肾衰合剂;质量标志物;非靶向代谢组学;网络药理学;含量测定

Screening and quantitative analysis of Q-Marker for anti-renal fibrosis of Shenqi shenshuai mixture based on untargeted metabolomics and bioinformatics

ZHOU Yuhang^{1,2}, LI Yuqi^{1,2}, GAO Zhuo^{1,2}, RUAN Qingfeng², ZENG Xiaoxuan², WANG Hui³, HUANG Chuanqi^{1,2}, XU Hongfeng^{1,2}[1. School of Pharmacy, Hubei University of Chinese Medicine, Wuhan 430065, China; 2. Dept. of Pharmacy, Wuhan No.1 Hospital, Wuhan 430022, China; 3. Hubei Center for Adverse Drug (Medical Device) Reaction Monitoring, Wuhan 430060, China]

ABSTRACT **OBJECTIVE** To screen and quantitatively analyze the quality marker (Q-Marker) associated with anti-renal fibrosis in Shenqi shenshuai mixture (SQSS), so as to provide references for the analysis of pharmacodynamic substances and new drug transformation of SQSS. **METHODS** The chemical components of SQSS were characterized by untargeted metabolomics. Combined with network pharmacology, gene expression omnibus (GEO) and connectivity map (CMAP) databases, the anti-renal fibrosis Q-Markers of SQSS were screened. HPLC-MS/MS was applied to determine the contents of Q-Markers in 10 batches of SQSS. **RESULTS** A total of 1 319 compounds were identified from SQSS via untargeted metabolomics, and 84 active ingredients with anti-renal fibrosis activity were further screened out, such as formononetin. Nine anti-renal fibrosis Q-Markers were obtained by network pharmacology and GEO database, including berberine, quercetin, honokiol, nicotinamide, daidzein, coumarin, kaempferol, formononetin and amygdalin. The quantitative results showed that the average contents of the above components (excluding amygdalin) in 10 batches of SQSS were 2.523, 1.942, 26.848, 1.415, 0.692, 0.171, 0.374, 7.401 μg/mL,

respectively. **CONCLUSIONS** Nine anti-renal fibrosis Q-Markers of SQSS were screened in this study, and the contents of eight among them were determined. The results can provide a basis for elucidating the pharmacodynamic material basis and promoting the new drug transformation of SQSS.

KEYWORDS Shenqi shenshuai mixture; Q-Marker; untargeted metabolomics; network pharmacology; content determination

^Δ基金项目 全国中药特色技术传承人才培养项目(No. 国中医药人教函[2023]96号);湖北省自然科学基金项目(No. 2026AFC1101);湖北省时珍人才工程项目(No. 鄂卫办发[2024]20号);武汉市卫生健康委青年人才资助“晨星计划”(No. 武卫发[2023]28号)

* 第一作者 硕士研究生。研究方向: 中药质量控制与分析。
E-mail: 2436836041@qq.com

通信作者 主任中药师, 硕士生导师。研究方向: 中药质量控制与新制剂开发。E-mail: 282215830@qq.com