



基于UPLC-PDA-MS/MS技术的四逆散水煎液体内外物质基础研究

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中文摘要:目的: 采用液质联用技术, 分析四逆散水煎液体外化学成分及血中移行成分, 对其体内外物质基础进行研究。方法: 采用ACQUITY UPLC™ BEH C₁₈柱 (2.1 mm×100 mm, 1.7 μm), 以乙腈-2 mmol·L⁻¹ 醋酸铵水溶液为流动相进行梯度洗脱, 流速0.2 mL·min⁻¹, 柱温35℃; 质谱采用ESI源, 正负离子同时检测, 在m/z 100-1 000进行扫描, 并对特征离子进行2次裂解, 获得二级质谱数据。结果: 在四逆散水煎液中, 检测到芍药苷、甘草酸、柴胡皂苷A及柚皮苷等20种化学成分。在体内样品中, 发现芍药苷、柚皮苷、橙皮苷等8种成分以原型入血, 同时还检测到6种代谢物, 包括葡萄糖醛酸结合物、硫酸酯结合物及葡萄糖醛酸硫酸酯结合物等。结论: 采用UPLC-PDA-MS/MS技术分析四逆散水煎液的体内外化学成分, 能比较全面、快速地反映四逆散水煎液的体内外物质基础, 为进一步研究四逆散的药效物质基础提供依据。

中文关键词: UPLC-PDA-MS/MS 体内外物质基础 四逆散水煎液 化学成分

Study on *in vitro* and *in vivo* material base of Sini San by UPLC-PDA-MS/MS

Abstract: Objective: To analyze chemical constituents of Sini San its migrating components in rat plasma and study its *in vitro* and *in vivo* material base using ultra-performance liquid chromatography coupled with photo-diode-array detector and tandem mass spectrometry (UPLC-PDA-MS/MS). Method: ACQUITY UPLC™ BEH C₁₈ column (2.1 mm×100 mm, 1.7 μm) was adopted, with gradient elution system of water containing 2 mmol·L⁻¹ ammonium acetate and acetonitrile at flow rate of 0.2 mL·min⁻¹. The column temperature was maintained at 35℃. The mass spectra were obtained by electrospray ionization source operating in both positive and negative ion mode. Ions were scanned from the m/z 100 to 1 000, and the characteristic ions were schizolysised twice to obtain the secondary MS data. Result: Twenty chemical constituents were detected, including paeoniflorin, glycyrrhizic acid, saikosaponins a and naringin. *In vivo*, there were 8 ingredients directly absorbed into blood after the administration of Sini San decoction, such as paeoniflorin, naringin and hesperidin. Besides, 6 metabolites were also detected, involving glucuronides, sulfate and sulfoglucuronides. Conclusion: *In vitro* and *in vivo* chemical materials of Sini San decoction is analyzed by UPLC-PDA-MS/MS to reflect *in vitro* and *in vivo* material base of Sini San decoction in a comprehensive and rapid manner and provide basis for further study on efficacious material basis of Sini San decoction.

keywords: UPLC-PDA-MS/MS *in vitro* and *in vivo* material base Sini San decoction chemical constituent

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