振阳救心汤治疗慢性心力衰竭的药效物质基础研究Δ

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摘　要　目的　分析振阳救心汤的化学成分及入血原型成分，挖掘其治疗慢性心力衰竭（CHF）的潜在活性物质。**方法**　将SD大鼠分为空白组（蒸馏水）以及给药0、15、30、60 min组（14.96 g/kg，以生药量计），每组2只。每12 h灌胃1次，连续3 d。末次给药后，采集大鼠血液并制备含药血清。采用超高效液相色谱-四极杆/静电场轨道阱高分辨质谱结合全球天然产物社群分子网络技术鉴定振阳救心汤的化学成分及含药血清中入血原型成分，并结合网络药理学、分子对接及分子动力学模拟预测其治疗CHF的潜在活性成分及作用靶点。**结果**　从振阳救心汤中共鉴定出化学成分116种，包括黄酮类（29种）、萜类（26种）、皂苷类（22种）等多种成分；在含药血清中共鉴定出淫羊藿苷、人参皂苷Rg_1、白术内酯Ⅰ等20种入血原型成分。通过网络药理学筛选，得到淫羊藿苷、人参皂苷Rg_1、白术内酯Ⅰ、十六酰胺等6个关键活性成分，以及糖原合成酶激酶3β（GSK-3β）、淀粉样前体蛋白（APP）、表皮生长因子受体（EGFR）等6个关键核心靶点。分子对接结果显示，关键活性成分与关键核心靶点间均具有一定结合活性，其中以淫羊藿苷与APP的结合能力最强；分子动力学模拟表明，淫羊藿苷与APP形成的复合物具有良好的稳定性。**结论**　振阳救心汤治疗CHF的潜在活性成分为淫羊藿苷、人参皂苷Rg_1、白术内酯Ⅰ等，作用靶点为APP、EGFR、GSK-3β等；其中APP可能为淫羊藿苷的重要作用靶点之一。

关键词　振阳救心汤；慢性心力衰竭；入血成分；分子网络；网络药理学；淫羊藿苷

Study on the material basis of efficacy of Zhenyang jiuxin decoction for the treatment of chronic heart failure

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ABSTRACT　OBJECTIVE To analyze the chemical constituents and absorbed prototype components in blood of Zhenyang jiuxin decoction, and explore its potential active substances in the treatment of chronic heart failure (CHF). **METHODS** SD rats were divided into a blank group (distilled water) and administration groups with blood collection at 0, 15, 30 and 60 min after dosing (14.96 g/kg calculated by crude drug), with 2 rats in each group. Intragastric administration was conducted once every 12 hours for 3 consecutive days. After the last administration, rat blood was collected to prepare drug-containing serum. UPLC-Q-Exactive Orbitrap HRMS combined with the Global Natural Products Social Molecular Networking technology was adopted to identify the chemical constituents of Zhenyang jiuxin decoction and the absorbed prototype components in blood in drug-containing serum. Moreover, network pharmacology, molecular docking and molecular dynamics simulation were used to predict the potential active components and action targets for CHF treatment. **RESULTS** A total of 116 chemical constituents were identified from Zhenyang jiuxin decoction, including flavonoids (29 species), terpenoids (26 species), saponins (22 species) and other compounds. Twenty absorbed prototype

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