[1]沈继斌,佟巍,崔颖,等.生物胶束色谱中黄酮类化合物定量保留-药动学性质预测模型的研究[J].第三军医大学学报,2013,35(12):1257-1261.
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生物胶束色谱中黄酮类化合物定量保留-药动学性质

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Title: Quantitative retention-pharmacokinetic activity relationship model of flavonoids by biopartitioning micellar chromatography

作者: 沈继斌; 佟巍; 崔颖; 李灵芝
天津医科大学药学院; 武警后勤学院药物化学教研室; 天津市职业与环境危害防治重点实验室

Author(s): Shen Jibin; Tong Wei; Cui Ying; Li Lingzhi
College of Pharmacy, Tianjin Medical University, Tianjin, 300070; Department of Pharmaceutical Chemistry, Logistics College of Chinese People's Armed Police Forces, Tianjin, 300162; Tianjin Key Laboratory for Prevention and Control of Occupational and Environmental Hazard, Tianjin, 300162, China

关键词: 生物胶束色谱; 定量保留-药动学活性关系; 黄酮

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摘要: 目的 利用生物胶束色谱（biopartitioning micellar chromatography, BMC）建立黄酮类化合物保留-药动学性质定量关系（quantitative retention activity relationship, QRAR）预测模型。 方法 测定化合物在pH=7.4的0.05 mol/L Brij 35缓冲盐流动相中的保留时间并计算保留因子，对保留因子与文献报道药代动力学参数进行拟合，建立QRAR模型，并对模型相关性和预测能力进行评价。 结果 在最佳流动相条件下，半衰期（$T_{1/2}$）、表观分布容积（Vd）和总清除率（Cl）的QRAR模型的相关系数分别为0.938、0.898和0.837，在置信度99%的水平上有统计学意义（$P<0.01$），模型标准差分别为41.929、19.528和0.139。交叉验证结果显示，模型校正集均方根误差(RMSEC)、交互验证均方根误差(RMSECV)、以内插值替换的交互验证均方根误差($RMSECV_i$)具有可比性，符合预测性能统计学要求。 结论 构建的黄酮类化合物药代动力学性质QRAR模型具有较好的相关性和预测性能。

Abstract: Objective To develop a quantitative retention-activity relationship (QRAR) model by biopartitioning micellar chromatography (BMC) for estimating the

pharmacokinetic parameters of flavonoids. Methods The retention time of the flavonoids in Brij 35 buffer solution (0.05 mol/L, pH 7.4) were determined, and the retention data of flavonoids and their corresponding properties were adjusted to a second-order polynomial QRAR model, of which the interpretative and predictive abilities were evaluated. Results The QRAR models of half-life period ($T_{1/2}$), apparent volume of distribution (Vd) and systemic clearance (Cl) obtained with the optimized chromatography conditions were statistically significant in the correlation coefficients, which were 0.938, 0.898 and 0.837 with the standard deviation of 41.929, 19.528 and 0.139, respectively. The comparability of cross validation results met the statistical requirement for good prediction. Conclusion The pharmacokinetic QRAR model obtained using the retention data of flavonoids shows good interpretative and predictive abilities.

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沈继斌, 佟巍, 崔颖, 等. 生物胶束色谱中黄酮类化合物定量保留-药动学性质预测模型的研究[J].第三军医大学学报,2013,35(12):1257-1261.