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论文

色谱指纹图谱定性相似度和定量相似度的比较研究

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摘要：

以药材栀子为例，对中药色谱指纹图谱定性相似度和定量相似度的宏观评价方法进行比较研究。用栀子对照药材和不同产地的栀子药材的HPLC指纹图谱实验结果，分别从化学成分分布相似性和含量相似性两个方面评价各产地药材与对照指纹图谱的相似性。以对照药材供试液不同进样量时获得的数据比较定性和定量相似度差异。提出了指纹图谱比率定性相似度s_F'，投影含量相似度*C*%、定量相似度*P*%和平均质量百分数*M*%等一系列概念。结果显示，表征化学成分分布相似性的定性相似度不能揭示含量性质，只有在定性相似度合格基础上，定量相似度合格的药材才能满足生产和实际需要。可见，定性相似度和定量相似度的密切结合是用指纹图谱宏观控制药材质量的最佳方法。

关键词： 比率定性相似度 投影含量相似度 宏观含量相似度 定量相似度 栀子 HPLC指纹图谱

Comparison between the qualitative similarity and the quantitative similarity of chromatographic fingerprints of traditional Chinese medicines

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Abstract:

To explore the differences between the qualitative similarity and the quantitative similarity of chromatographic fingerprints of traditional Chinese medicines, the quantitative similarity calculated by vector shadow *C*%, apparent quantitative similarity *r*%, quantitative similarity *P*%, etc. were firstly proposed to disclose the quantitative information characteristics of traditional Chinese medicines fingerprints. The HPLC fingerprints of both the standard *Fructus gardeniae* and the ten batches of *Fructus gardeniae* produced in different places were evaluated by the new parameters to obtain good results. The contrasted fingerprint contained 35 peaks while geniposide was selected as the reference peak. The HPLC fingerprint had good precision and reproducibility with the RSD of the relative retention time less than 1.5% and the RSD of the relative peak area within 5%. The qualitative similarity and quantitative similarity between each crude drug and the contrasted fingerprint were quantitatively calculated, the values of *C*%, *P*%, etc., were applied in the quality control practice, which had less errors. What is more, this method could be used for the overall quality control of *Fructus gardeniae* and especially suits for qualitative and quantitative evaluations of the chromatographic fingerprints both in chemical constituent distribution and in contents. The quantitative parameters such as *C*% and *P*% can be used to objectively, authentically and thoroughly display the content information characteristics. When they combined with the qualitative similarity, it will be the good method to evaluate the chromatographic fingerprints of traditional Chinese medicines.

Keywords: quantitative similarity calculated by vector shadow *C*% apparent quantitative similarity *r*% quantitative similarity of *P*% *Fructus gardeniae* HPLC fingerprints qualitative similarity of peak area ratio

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