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ΔSr等级序列模式识别法分析补中益气丸和十全大补丸HPLC指纹图谱

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摘要：

建立一种新的中药HPLC指纹图谱模式识别方法-指纹图谱相对峰面积差（ΔSr）等级序列模式识别法，可以综合利用指纹峰峰位定性信息及成分含量信息实现中药复方黑箱体系的鉴别及定量质量评价。测定了中药复方补中益气丸和十全大补丸无水乙醇提取物HPLC指纹图谱，建立ΔSr序列。根据正态分布定义不同相似度等级ΔSr≤ΔSr+xSv,-3≤x≤+3, 确定各样品的特征样品组,构成每个样品的分类信息。该法无须对照样品及经验知识,可以对这两种组成相似的中药复方进行准确精细的分类,品种识别率100%,而相关系数r和向量夹角余弦cosα相似度法无法准确识别两类样品。ΔSr等级序列聚类法是一种准确的HPLC指纹图谱分析方法,适用于中药复方复杂生物系统-一种黑箱系统的鉴别及质量评价。

关键词： 补中益气丸 十全大补丸 指纹图谱 &Delta Sr序列 鉴别 模式识别 黑箱

HPLC fingerprint spectra analysis of Buzhong Yiqi Pills and Shiquan Dabu Pills by the relative peak area difference ΔSr

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Abstract:

An efficient and simple pattern recognition method relative peak area difference (ΔSr) grade sequence classifying method was established. It is suitable for analyzing HPLC fingerprint spectra of herbal medicines Buzhong Yiqi Pills and Shiquan Dabu pills based on both information of peak positions and contents of compounds, and it is qualified to recognize the two traditional Chinese compound formulae which are so-called “black box” systems. The HPLC fingerprint spectra of these two medicines’ components extracted with absolute ethanol were measured, and the ΔSr sequences of these samples were constructed. Then their most similar sample groups characteristic sequences named ΔSr grade sequences were determined depending on the similarity scale ΔSr≤ΔSr+xSv,-3≤x≤+3. In addition, clustering and classification of these samples were performed relying on the characteristic sequences. These two kinds of medicine were accurately and subtly recognized by this new method, with the correct ratio of 100%. The results were greatly superior to those obtained by means of coefficient r and vectorial angle cosine(cosα) methods. The results also indicated that the ΔSr grade sequence clustering / classifying method was an accurate and simple approach suitable for quantitative identification and quality control of traditional Chinese compound formula, a kind of complex “black box” system.

Keywords: Buzhong Yiqi Pill Shiquan Dabu Pill fingerprint spectra ΔSr grade sequence identification pattern recognition black box

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参考文献：

本刊中的类似文章

1．赵然杭,陈守煜 .水资源数量与质量联合评价理论模型研究[J]. 山东大学学报(工学版), 2006,36(3): 46-50

2．李 莹,宋 刚 .汉字笔迹鉴别中预处理算法实现[J]. 山东大学学报(工学版), 2007,37(2): 80-83

3．林爱华 蒋晓芸 苗风明.粒子入射双δ势垒时空间分数阶薛定谔方程的解[J]. 山东大学学报(工学版), 2010,40(1): 139-143

4．孙文章,曹升乐 .东昌湖水质评价分析[J]. 山东大学学报(工学版), 2007,37(6): 95-97

5．董凤娟,邹华彬*,陆玮洁,杜爱琴.双指标等级序列模式识别法分析十全大补丸氯仿提取物红外指纹图谱[J]. 山东大学学报(工学版), 2010,40(6): 113-119

6．邹华彬1, 王丽双1, 翟红2.N-生物系统双指标等级序列个性化模式识别法及左归丸、右归丸和济生肾气丸核磁共振指纹图谱分析[J]. 山东大学学报(工学版), 2012,42(4): 114-119

7．何荣福1,肖民卿2*.圆形区域极点约束下的δ算子时滞系统鲁棒L2-L∞控制[J]. 山东大学学报(工学版), 2013,43(1): 69-79