

化学与化工

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

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摘要:

采用一种新型模式识别方法——双指标等级序列模式识别法,对不同厂家生产的中药复方十全大补丸样品氯仿提取物的红外指纹图谱进行了分析,以实现中药复方的准确鉴别及质量控制。该法同时具有无监督及有监督模式识别的优点,无须经验知识,通过确定每个样品双指标序列中的相似样品序列,同时进行聚类及分类分析。采用该法对3个不同厂家生产的22个中药复方中成药十全大补丸样品的氯仿提取物的红外指纹图谱进行鉴别研究,正确识别率达100%,而采用UPGMA系统聚类方法的正确识别率仅为72.7%。双指标等级序列模式识别法结合红外指纹图谱,无需任何先验知识即可实现中药复方的快速准确鉴别及质量评价。

关键词: 指纹图谱 聚类分析 模式识别 十全大补丸 鉴别

The dual index grade sequence pattern recognition method for analyzing infrared fingerprint spectra of extracts with chloroform of Shiquan Dabu Pills

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Abstract:

A new type identification method, dual index grade sequence pattern recognition method, was applied for identification and quality evaluation of the traditional Chinese compound formula Shiquan Dabu Pills produced by different companies. This approach possessed the advantages of both supervised and unsupervised pattern recognition methods, which could simultaneously cluster and classify the complex biological samples without prior knowledge. In the process, the most similar sample sequence of each sample was determined depending on common peak ratio index of samples and normal distribution. Similar samples should have 'most similar sample sequences', by which the samples could be efficiently recognized. The identification and quality evaluation of components of 22 Shiquan Dabu Pill samples produced by three companies extracted with chloroform were carried out by this novel approach and their infrared fingerprint spectra. The correct recognition rate of the samples was 100%, while it was only 72.7% by a famous hierarchical clustering method, an unweighted pair-group method using arithmetic averages (UPGMA). The results showed that the dual index grade sequence pattern recognition method together with infrared fingerprint spectra could accurately and simply finish the identification and quality estimation of the traditional Chinese compound formula, without any prior knowledge related to the analyzed samples.

Keywords: fingerprint spectra clustering analysis pattern recognition Shiquan Dabu Pills identification

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