研究论文

自动化色谱谱图解析——谱峰的自动识别与快速解析

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摘要　　结合基于高阶导数的谱峰识别方法和面积重现法, 建立了一种完全自动化的对色谱曲线进行分割、识别与快速解析的方法。其中, DW(Durbin-Watson)测试的引入和区分信号与噪声判据的采用减少了在色谱解析过程中的人为干预, 降低了对操作人员专业知识和经验的要求, 为实现色谱解析的自动化奠定了基础。通过对模拟色谱和实验色谱的比较, 验证了该方法是一个很有用的工具, 可以为色谱分析工作提供有力的帮助。

关键词　　面积重现法　谱峰识别　色谱解析　DW测试

Automatic peak recognition and rapid resolution of chromatographic signals with a self-compiling program

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Abstract

Area reproduction method was introduced in combination with peak recognition algorithm based on high-order derivatives to automate the chromatogram division, peak recognition and rapid resolution. Durbin-Watson method and the criterion to distinguish the signal and noise were adopted to reduce the user interaction. The objective was that the operators should be able to perform this method with minimal experience and professional knowledge. The method is a useful tool by applying it to the resolution of model and real chromatographic signals.

Key words　area reproduction　peak recognition　resolution of chromatographic signals　Durbin-Watson method

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