

论文

一种新软件方法用于单位分辨质谱仪上药物相对分子质量的准确测定

刘可;马彬;王永东;陈笑艳;钟大放

1. 中国科学院 上海药物研究所, 上海 201203; 2. Cerno Bioscience, Danbury, CT 06810, USA

摘要:

关键词: 准确相对分子质量 同位素 单位分辨质谱仪

A new software method for accurate mass measurements of drugs on unit mass resolution mass spectrometer

LIU Ke; MA Bin; WANG Yong-dong; CHEN Xiao-yan; ZHONG Da-fang

Abstract:

Accurate mass measurements of 20 drugs were conducted using MassWorks software on a TSQ Quantum Ultra mass spectrometer. All Q1 scan mass spectral data were collected in profile mode with full width at half-maximum (FWHM) set at 0.7 Da. The mass errors of all 20 drugs (molecular weight between 135 and 810) were within the range from -22.4×10^{-6} to 36.1×10^{-6} , among them 90% of the drugs achieved a mass accuracy better than 10×10^{-6} . The new method can provide accurate mass measurements on unit mass resolution mass spectrometers.

Keywords: isotope unit mass resolution mass spectrometer accurate relative molecular mass

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作者简介:

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