

ABSTRACT

Basic Information

Abstract Number: 830-4

Author Name: Yongdong Wang

Affiliation: Cerno Bioscience

Session Title: Advances in LC-MS Strategies for the Identification of Impurities, Degradants, and Metabolites

Event Type: Organized Contributed Session

Event Title: Calibrating Mass Spectrometers for Full Spectral Search

Presider(s): Lee, Mike

Start Time: 09:30 AM (Slot # 4)

Date: 03/14/2006

Location: 208A

Keywords: Liquid Chromatography/Mass Spectroscopy, GC-MS, Mass Spectrometry, Statistical Data Analysis

Co-Authors

Name

Affiliation

Gu, Ming

Cerno Bioscience

Abstract Content

The state-of-the-art in mass spectral data acquisition and mathematical processing requires raw mass spectral data be preprocessed before any library search or quantitation. The preprocessing steps include smoothing, de-isotoping or centroiding, and identifying and correcting for multiple charges, i.e., to reduce the raw continuous mass spectral data into "clean" stick spectrum. While these preprocessing steps vary from instrument to instrument and from vendor to vendor, they are all prone to algorithm-specific errors (biases) and they all cause a severe loss of information in the process, as mass spectral instrument profile would be completely lost and distortions in isotope abundances occur regularly. Due to the large errors associated with the mass spectral peak picking/centroiding, a large enough mass window has to be specified for the library search, another rather arbitrary and nonlinear cutoff introduced into the process. On a unit mass resolution system, a mass search window of $\pm 0.5\text{Da}$ is typically required due to the poor mass accuracy, resulting in too many hits to be useful for most applications, except for the cases where many fragments are available from the same parent ion for identification, such as LC/MS/MS peptide sequencing or GC/MS compound identification in the EI mode. A new full spectral calibration approach will be presented in this paper that avoids the centroiding process all together and thereby preserves the data integrity of mass spectral scans. The mass spectral data thus processed would not only have been noise-filtered but also mass calibrated to high mass accuracy in the full profile mode, allowing for accurate compound identification and ion chromatogram filtering in the presence of complex matrices even at unit mass resolution. The attached graph shows the identification and filtering of the extracted ion chromatogram for demethylation metabolites of Verapamil in a complex bile matrix.