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Cerno Bioscience Paper Demonstrates Accurate Mass Measurements from Product Ions on Unit Mass Resolution Mass Spectrometers

Danbury, CT. (July 24, 2006) – A new paper from Cerno Bioscience and Wyeth Pharmaceuticals, called 'Accurate Mass Measurements of Product Ions for Metabolite Identification on Unit Mass Resolution Mass Spectrometers', demonstrates that high mass accuracy can be achieved on conventional triple quadrupole mass spectrometers of unit mass resolution running in MS/MS mode. This is achieved using Cerno's award winning MS calibration and data analysis software, MassWorks™, an easy-to-use post acquisition software package that utilizes Cerno's patented MSIntegrity™ technology, to dramatically improve mass spectral measurements.

The level of accuracy required for metabolite identification can normally only be performed on high resolution mass spectrometers, but the results of this research prove that MassWorks can achieve mass measurements of product ions with 5 ppm accuracy on a unit mass resolution instrument.

The method was demonstrated for a set of small-molecule pharmaceuticals from an ABI/Sciex 4000 Q Trap by infusion as well as by LC/MS/MS measurements of rat liver microsomal incubation of verapamil on an ABI/Sciex 3200 Q Trap. All the mass spectral data were collected in profile mode and processed using MassWorks software.

For the infusion, a few or a single known fragment ion(s) from the MS/MS spectra were selected as calibration standards in order to internally calibrate the spectra. Other fragment ions in the spectra were tested for mass accuracy resulting in mass errors of less than a few mDa in most cases.

The LC/MS/MS fragment ions were generated on-the-fly by information dependent scans. Accurate mass measurements of about 5 mDa for demethylated verapamil and its fragments were achieved by applying an external calibration generated by the known fragments of the parent drug verapamil.

Interestingly, the research also found that mass spectrometry calibration, including both mass and peak shape, is critical for high mass accuracy and that internal calibration aids the achievement of the highest possible mass accuracy. Peak saturation is a key factor causing poor mass accuracy in a quadrupole system.



MassWorks recently won the PITTCON 2006 Editors' Choice Bronze Award following its show debut at the Pittsburgh Conference of Analytical Chemistry and Applied Spectroscopy in March 2006. This prestigious accolade is given to the best new product introduction for its contribution to the advancement of science, as judged by a panel of editors attending the show.

MassWorks utilizes Cerno's DirectRead™ technology to read most instrument data formats directly, eliminating the need for importing or exporting MS data to the clipboard or utilizing intermediate exchange formats. This saves time, reduces transcription errors, simplifies file management, and saves substantial disk space. As DirectRead doesn't alter the original data, it assists compliance with common regulatory requirements such as GLP and 21 CFR Part 11.

To access the research paper please visit www.cernobioscience.com/resources
For more information on MassWorks, please contact Cerno Bioscience at info@cernobioscience.com, call +1 203-312-1150, or visit www.cernobioscience.com

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About Cerno Bioscience LLC

Cerno is dedicated to the practical application of modern mathematical techniques to Mass Spectrometry for the purpose of improving the quality, accuracy and reliability of MS analysis. These techniques can be used to dramatically improve the amount of information obtainable from and reduce the amount of time required of many MS experiments. Cerno's technologies are proprietary and protected through numerous patents granted and submitted world-wide. The company was founded and is staffed by a team with over 80 years' experience in the fields of instrumentation, mathematical data processing, life science applications and biotech business development. Cerno is funded by a private investment group with an established track record of success in the Analytical Instrumentation market.