

## Cerno Bioscience Announces Journal Publication of MassWorks™ sCLIPS Application to High Resolution MS

**Danbury, CT., (August 4, 2010)** – Cerno Bioscience has today announced a user publication in the Journal of the American Society for Mass Spectrometry (JASMS) on the application of its award-winning MassWorks™ software to high resolution MS systems. Better known for its 100x improvement in mass accuracy, unparalleled Spectral Accuracy, and the uniquely enabled formula determination capability on unit mass resolution quadrupole system, MassWorks, with the added sCLIPS™ feature, extends the concept of Spectral Accuracy to high resolution MS systems such as TOF, qTOF, or FTMS to further reduce the number of possible formula candidates obtained through the more widely used mass accuracy.

In this JASMS article, three different approaches of utilizing the important isotope information for formula determination were systematically reviewed and compared. These include the simplistic isotope ratio measurement based on centroid data, what appears to be a fitting statistic based on un-calibrated profile mode data, and the most advanced Spectral Accuracy based on peak-shape-calibrated profile mode data capable of mathematically exact isotope modeling. According to the results reported in the article by this pharmaceutical industry user on the study of a comprehensive list of large molecules with m/z extending beyond 1000Da, there are typically over a hundred or more formula candidates within the mass tolerance window of 5ppm or even 1ppm. Not only can the use of Spectral Accuracy eliminate 99% of incorrect formula candidates, it can also be used to monitor and optimize the MS operating conditions. For example, this study pointed out the optimal resolving power in terms of Spectral Accuracy is around 15,000:1 on the ThermoFisher Scientific Orbitrap FTMS instrument. With the high Spectral Accuracy achieved, it is possible to separate mass spectrally overlapping ion signals for exact mixture analysis, such as the case involving an ion pair created by the loss of two hydrogen atoms, which may be difficult to separate through either chromatography or high resolution MS. For more details, please read the complete article at <http://dx.doi.org/10.1016/j.jasms.2009.07.014>.

### About Cerno Bioscience Products

Cerno Bioscience's MassWorks family of software products performs post-acquisition MS calibration and formula determination through either CLIPS at unit mass resolution or sCLIPS at higher resolution. It supports all major MS vendor data formats and works with all MS instruments including GC/MS, LC/MS, TOF, qTOF, and FT MS. Cerno Bioscience products are used in major R&D labs for pharmaceuticals, food, beverages, flavors, fragrances, natural products, environmental analysis, forensics, fine chemicals and petrochemicals. For more information, please visit: <http://www.cernobioscience.com/products.html>.

### About Cerno Bioscience

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. For more information on Cerno MS technologies, applications, or products please visit our Web site:

[www.cernobioscience.com](http://www.cernobioscience.com).

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