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Cerno Bioscience and SABIC Innovative Plastics Demonstrate Accurate Formula ID by Spectral Accuracy Using Ion Trap Mass Spectrometer

Danbury, CT. (January 30, 2008) – Cerno Bioscience in cooperation with Dr. Christian Wold of SABIC Innovative Plastics have succeeded in demonstrating the ability to perform formula ID on a Thermo LCQ Deca Max ion trap mass spectrometer.

Using MassWorks™ sCLIPS (Self Calibrated Lineshape Isotope Profile Search), the latest addition to the MassWorks mass spectrometry software suite, the researcher was able to ID a set of trial compounds to within a top few compounds from a list of hundreds of formula candidates. MassWorks was originally launched in 2006, and received the prestigious Editors' Choice Bronze Award at PITTCON 2006. MassWorks is an easy-to-use post acquisition software system using Cerno's patented MSIntegrity calibration technology to work directly with data from a wide range of mass spectrometers.

Formula ID normally requires accurate mass measurements typically provided high resolution Time-of-Flight (TOF), Orbitrap, or FT-ICR instrumentation. Ion traps typically cannot provide accurate mass measurements due to physical limitations of the ion trap analyzer, particularly in the older 3D trap designs such as the instrument used in this study. However, the studies here have shown that by carefully controlling the ion trap conditions, it is possible to attain high spectral accuracy which is suitable in itself for Formula ID. The approach utilizes Cerno's sCLIPS to correct the instrument line-shape and allow highly accurate matching of the isotope pattern of the unknown ion against theoretically calculated ion candidates. One of the benefits of the approach is that it requires no known calibration ions, and instead utilizes the ion traps ability to scan in high resolution mode to resolve the isotope peaks. The monoisotopic peak of the analyte ion can then be used to correct the isotope line-shape pattern for accurate matching to theoretical spectra.

Ming Gu, VP of Research for Cerno notes "We were quite surprised by the level of performance achievable on the 3D trap design. This work is a good indication that even better results should be obtainable with more modern linear ion trap designs". The approach extends the versatility of ion trap instruments by enabling them to provide formula identification, a capability previously not though possible.

For more information on MassWorks CLIPS, please email 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.