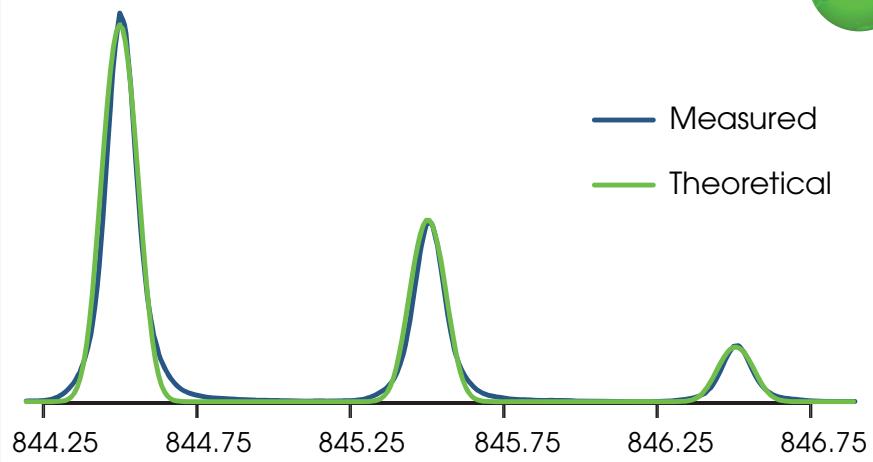
MassWorks™

Revolutionary software for
MS calibration and formula ID

Now with solutions for both High Resolution and Unit Resolution mass spectrometers

Building on the success of its award winning **MassWorks MS** data processing software, Cerno is proud to announce the latest breakthroughs for extending the capabilities of any mass spectrometer. Whether you use unit resolution quadrupole systems for GC or LC/MS or any high resolution system from TOF to FT-MS, MassWorks can enable or enhance your ability to perform formula ID as well as to easily obtain higher quality, more reproducible data from your current instrument. MassWorks is an easy-to-use post acquisition software package utilizing Cerno's patented **MSIntegrity** calibration technology that works directly with data acquired from most popular mass spectrometers. Simply acquire the data using your current MS data system and then just open, process, and report from MassWorks. In addition to directly reading native data from major MS vendors, MassWorks now also imports ASCII data from your current software via cut and paste or exported ASCII files allowing it to work with virtually any make or model of mass spectrometer.

Increase your productivity and improve your confidence to correctly identify unknown formula



NEW!

For high resolution MS, such as TOF, OrbiTrap, or FTMS, dramatically improve your ability to uniquely identify unknown formula from the long list of possible formula candidates obtained by mass accuracy alone, without the need for calibration standards!

For quadrupole LC/MS or GC/MS, perform accurate formula ID on these otherwise conventional MS systems with up to 100x better mass accuracy.

MassWorks also improves the quality of data from any mass spectrometer by improving the reproducibility, signal-to-noise, and MS peak detection.

MassWorks™ Spectral Accuracy is a measure of the similarity between the measured isotope pattern (ion spectrum) and the theoretical ion spectrum. Without proper line-shape calibration, Spectral Accuracy values are of limited use in differentiating closely related formulas.

FROM MASS ACCURACY TO SPECTRAL ACCURACY

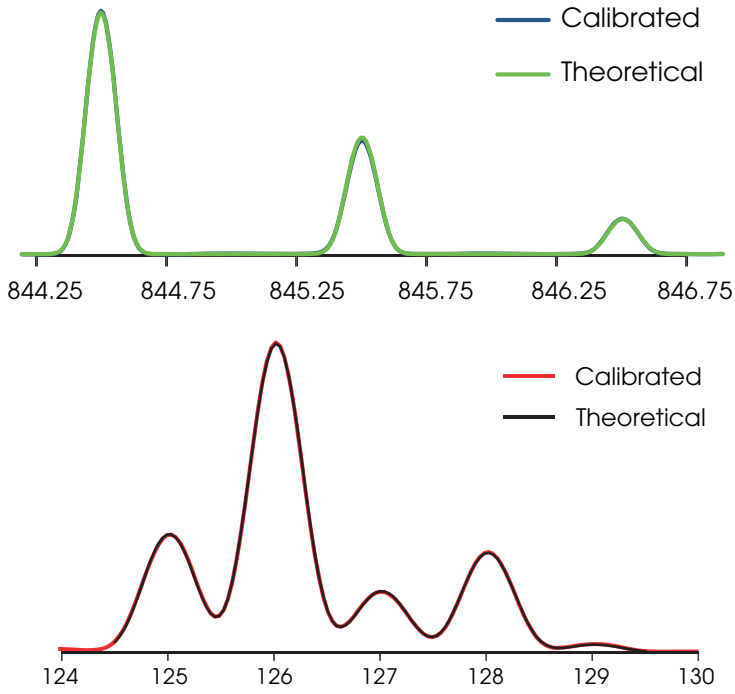
Mass Accuracy is a measure of an instrument's error in determining the theoretical (exact) mass of an ion and is usually expressed in parts-per-million (ppm) relative to the exact mass values or in absolute units of milli-Daltons (mDa). Unfortunately, due to the presence of many possible formulas conforming to a given mass measurement error, mass accuracy alone can rarely provide a unique formula, particularly at higher mass values (above 400Da). For example, even FT-ICR with 1 ppm mass accuracy makes you choose from 569 possible formulas at 477.2303 Da with the common organic elements C, H, N, O, S, Cl, P, F, and Na. Spectral Accuracy is a measure of the similarity between the measured spectrum

(the entire ion isotope pattern) against that of the theoretical spectrum. However, since the line-shape of the measured spectrum is unknown and instrument/MS tune dependent, measures of Spectral Accuracy are generally not high enough to provide a unique formula. Cerno's MassWorks software elegantly addresses this problem by not only accurately calibrating the mass position of the peak, but by also calibrating the MS line-shape to a mathematically defined function. This allows extremely accurate comparisons to be made between the calibrated and theoretical spectra with Spectral Accuracy values capable of uniquely identifying an unknown ion formula. This patented, powerful approach to formula ID is called **CLIPS** (Calibrated Line-shape Isotope Profile Search) for low resolution instruments and **sCLIPS** (self Calibrated Line-shape Isotope Profile Search) for higher resolution instruments.

CLIPS™

sCLIPS™

MassWorks software calibrates for spectral line-shape as well as for mass position allowing highly accurate comparisons between calibrated and theoretical spectra with Spectral Accuracy as great as 99.9%. This greatly enhances formula ID on higher resolution instruments, and, when combined with the improved mass accuracy of the MassWorks calibration, enables formula ID on unit resolution GC and LC/MS quadrupole instruments.



Accurate spectral overlay for CLIPS search of the GC/MS spectrum of 4-chlorotoluene (C_7H_7Cl nominal mass 126 Da). MassWorks correctly identifies the compound with a Spectral Accuracy of 99.5% and a mass accuracy of 9 ppm despite interference of the M-H ion at 125 Da, a common problem in GC/MS, but is easily compensated for by using MassWorks mixture search feature.

FOR ACCURATE MASS INSTRUMENTS

Enhance formula ID accuracy using this calibrant-free method for higher resolution instruments with sCLIPS

APPLICABLE FOR - TOF, QTOF, HIGH RESOLUTION QUADRUPOLES, ORBITRAP, OR FTMS.

sCLIPS searches are simple and easy to perform, with no calibrant required. This relaxes the need to perform the sometimes tedious and time consuming protocols to obtain accurate mass measurements. This can save you time and increase your sample throughput, while improving your results as well. Simply open the data file directly into MassWorks, or cut and paste from your instrument vendor software, click on the monoisotopic peak label to launch sCLIPS, and the calibration is automatically performed and the search results returned.

FOR UNIT RESOLUTION QUADRUPOLE INSTRUMENTS

Obtain accurate mass and perform formula ID on unit resolution GC/MS and LC/MS with single and triple-quadrupoles through CLIPS

APPLICABLE FOR – SINGLE AND TRIPLE QUAD GC/MS AND LC/MS INSTRUMENTS

Dramatically improve both the mass accuracy and Spectral Accuracy to enable formula ID on these otherwise conventional MS systems. By using known calibration compounds and the MassWorks patented MSIntegrity calibration, it is possible to routinely obtain mass accuracy in the 5-10mDa range. This, combined with the high Spectral Accuracy achieved through the MassWorks line-shape calibration, allows for confident formula ID.

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FOR MORE INFORMATION
visit our website at **www.cernobioscience.com**
or email to **info@cernobioscience.com**
14 Commerce Drive • Danbury, CT 06810 • USA • Tel 1-203-312-1150