Introducing...

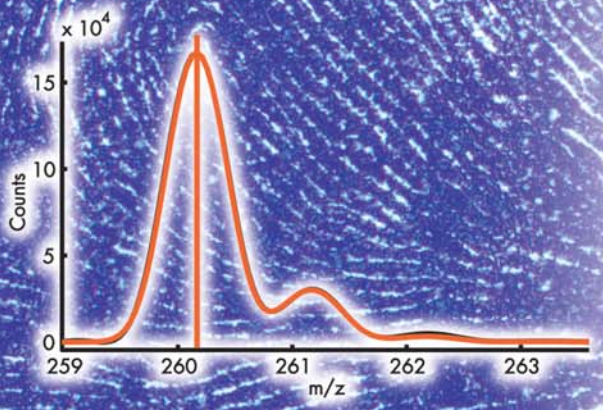
MassWorks™ CLIPS™

A revolutionary approach for obtaining fast and reliable Formula ID from any single or triple quadrupole Mass Spectrometer

Formula ID From Your Quadrupole!

Mass Accuracy PLUS Spectral Accuracy!

- ✓ Provides 2 dimensions for Formula ID
  - Mass Accuracy to 5ppm
  - Spectral Accuracy to .1%
- ✓ Improved signal-to-noise (3X)
- ✓ Works with Thermo, AB/Sciex, Waters, Agilent, and more MS systems



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Formula	Mass Error (mDa)	Spectral Accuracy
$C_{16}H_{22}NO_2$	-1.9	99.71
$C_{14}H_{20}N_4O$	-0.5	99.48
$C_{12}H_{18}N_7$	0.8	99.15
$C_{17}H_{24}S$	3.3	98.99

CLIPS (Calibrated Lineshape Isotope Profile Search) is an entirely new approach for obtaining elemental composition determination (ECD or sometimes called Formula ID) by utilizing both the high mass accuracy and spectral accuracy made available with Cerno's MassWorks calibration software. Performing Formula ID traditionally requires the use of expensive, highly specialized high resolution instruments combined with extensive calibration standards to provide accurate mass measurements. Formula ID is then performed using the accurate mass information to identify a list of formula candidates. But even with very high mass accuracy, the list of formula candidates can make unambiguous formula determination difficult.

Unlike approaches that use only mass accuracy for Formula ID, CLIPS adds another dimension of Formula ID by matching the full isotope profile of the unknown to the theoretical profile. In the past this has not been possible due to the uncalibrated line shape in mass spectrometry. This is now possible with Cerno's Patented MSIntegrity calibration technology that is available in its MassWorks™ software which calibrates for both mass accuracy as well as spectral accuracy.

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HOW DOES IT WORK?

CLIPS builds on the accurate mass calibration that MassWorks provides by using the full isotope fingerprint to unambiguously identify an unknown compound formula. The MassWorks patented calibration technology allows for accurate mass determination on typical unit mass resolution systems such as single and triple quadrupoles. Normally, these instruments produce results only to unit mass resolution, but with MassWorks, they can obtain up to 5ppm or better mass accuracy. This allows for a formula search to identify formula candidates just like with high resolution systems. However, the MassWorks calibration not only calibrates these instruments to accurate mass, it also calibrates for spectral accuracy by calibrating the actual instrument line shape to a known mathematical function. This allows for the accurate calculation of the theoretical isotope profile for each formula candidate using the same line shape as the calibrated line shape. The CLIPS algorithm then matches each formula candidate to the unknown and calculates a highly reliable statistic which is typically good to within a few tenths of one percent relative error, a level of spectral accuracy necessary to differentiate candidate formulas and arrive at unambiguous formula determination.

WHO CAN BENEFIT THE MOST FROM CLIPS?

MassWorks with CLIPS provides the most value to users of single and triple quad instruments. These instruments are renowned for their reliability, cost advantage, ease-of-use, versatility for use with various types of compounds, high sensitivity, and even portability or at least transportability. However, since they were considered only able to produce unit mass resolution data, were not considered for ECD of unknown compounds. MassWorks with CLIPS now greatly extends and expands the capabilities of these instruments into application areas never before possible.

For users without access to high resolution instruments, such as qTOF or FT-MS instruments, they now have the capability to perform ECD to assist in their unknown compound identification. Prior to this, the only choices were to send out the compound to other labs for further analysis, or, in the case where ample amounts of the unknown were available, attempt to perform a multitude of tests using a variety of analytical techniques.

For users with access to high resolution systems, it can provide inexpensive and routine ECD on a daily basis using simple, less expensive equipment. This frees up the high resolution systems and their highly trained operators for more challenging tasks. In addition, ECD can now be performed more routinely by less experienced operators to gain increased knowledge and more confidence on all measurements.

DOES IT WORK WITH OTHER TYPES OF INSTRUMENTS/DATA?

CLIPS provides greater confidence in ECD measurements for high resolution systems as well. Although high mass accuracy plays a significant role in reducing the number of formula candidates, the mass accuracy alone often fails to provide sufficient specificity to uniquely determine an unknown formula, even at a very high mass accuracy of 1 ppm. For example, an elemental search for hydroxylated buspirone resulted in three different possible formulas, $C_{21}H_{32}N_5O_3$ (1 ppm), $C_{21}H_{42}NP_2S$ (-1 ppm), and $C_{20}H_{38}N_3FPS$ (0.2 ppm) where the formula with what appears to be the highest mass accuracy turns out to be the wrong formula. However, by using CLIPS, the isotope profile enables unambiguous identification of the correct formula.

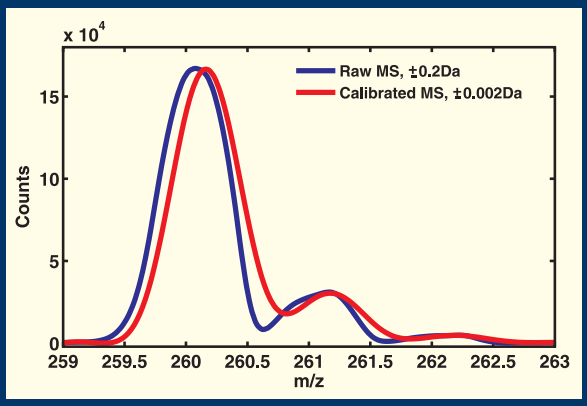

Figure 1 The patented MassWorks calibration not only provides for high mass accuracy, but high spectral accuracy as well. Because the line shape is calibrated to a known function, it is now possible to compare it with unprecedented accuracy to theoretical spectra using the same calibrated line shape.

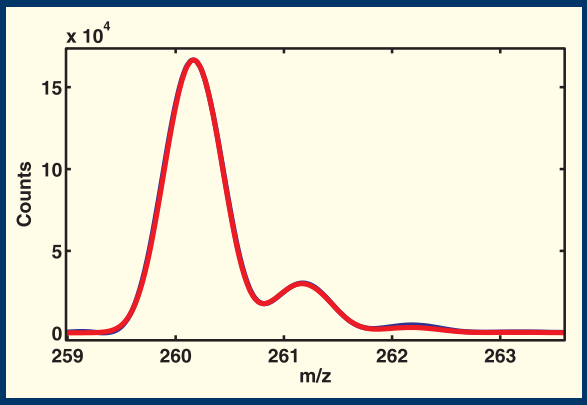

Figure 2 The CLIPS match of the MassWorks calibrated spectrum (Red) against the calculated theoretical spectrum of $C_{16}H_{22}NO_2$. The spectral accuracy match unambiguously identifies this unknown compound.

Formula	Mono Isotope	Mass Error (mDa)	Mass Error (PPM)	Spectral Accuracy
$C_{16}H_{22}NO_2$	260.1651	-1.9	-7.1	99.71
$C_{17}H_{24}O_2$	260.1776	-14.4	-55.5	99.65
$C_{15}H_{22}N_{3O}$	260.1763	-13.1	-50.3	99.63
$C_{15}H_{20}N_2O_2$	260.1525	10.7	41.2	99.59
$C_{14}H_{20}N_{4O}$	260.1637	-0.5	-2	99.48
$C_{13}H_{20}N_6$	260.1749	-11.7	-45.1	99.35
$C_{13}H_{18}N_{5O}$	260.1511	12.1	46.4	99.27
$C_{12}H_{18}N_7$	260.1624	0.8	3.2	99.15
$C_{16}H_{22}NS$	260.1473	15.9	61.1	99.06
$C_{17}H_{24}S$	260.1599	3.3	12.8	98.99
$C_{19}H_{18}N$	260.1439	19.3	74.1	98.97
$C_{11}H_{16}N_8$	260.1498	13.4	51.5	98.92
$C_{13}H_{24}O_5$	260.1624	0.8	3.2	98.79

Figure 3 While the MassWorks calibration provides excellent mass accuracy, the mass accuracy alone is not sufficient to uniquely identify the target compound ($C_{16}H_{22}NO_2$). However, the CLIPS isotope profile match uniquely establishes the compound ID using the spectral accuracy.

Extending the limits of mass spectrometry

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