

CLIPS Product Preview

What is it?

CLIPS is an entirely new and revolutionary way to attain fast and reliable elemental composition determination (ECD) from any single or triple quadrupole Mass Spectrometer. ECD is a powerful tool to assist in the identification of unknown compounds. ECD traditionally requires the use of expensive, highly specialized high resolution instruments combined with extensive calibration standards to provide accurate mass measurements. ECD 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 ECD, 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 unknown line shape in mass spectrometry. This however, is now made not only possible but highly accurate by using Cerno's MSIntegrity calibration technology that is available in its MassWorks™ software.

What does CLIPS stand for?

CLIPS is a descriptive acronym for Calibrated Lineshape Isotope Profile Search.

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 such as is done on high resolution systems. However, the MassWorks calibration not only calibrates these instruments to accurate mass, it also calibrates 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 with typically less than 1% relative error, a level of profile accuracy necessary to differentiate candidate formulas and arrive at unambiguous formula determination, even on a unit mass resolution system such as a single quadrupole MS.

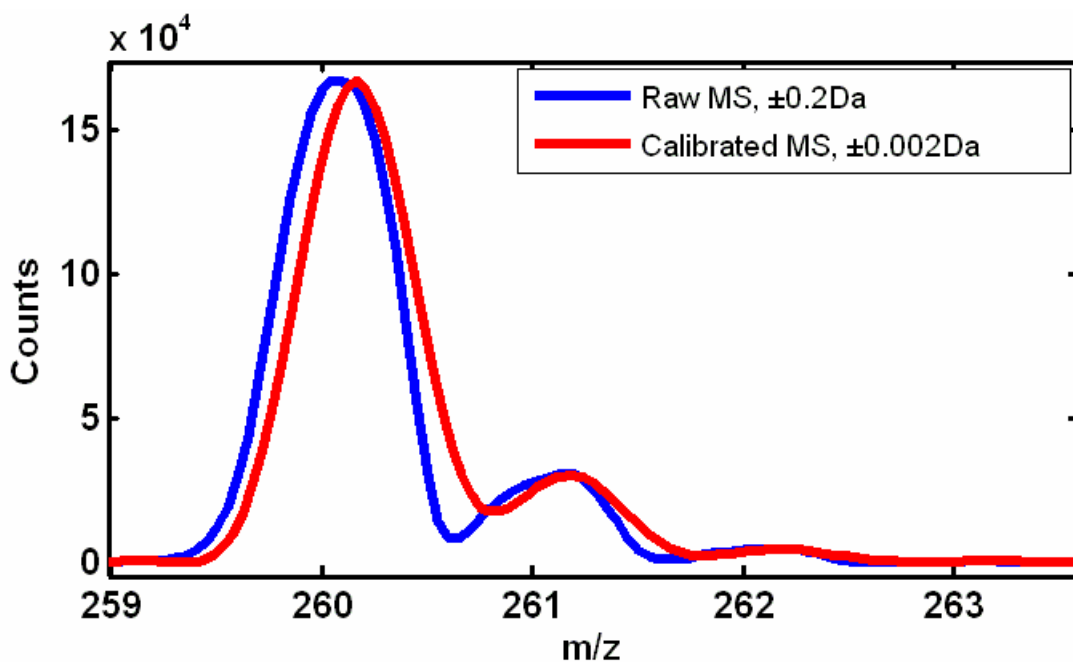


Figure 1 The patented MassWorks calibration not only provides for accurate mass calibration, but the line shape is calibrated as well. Because the line shape is calibrated to a known function, it is now possible to compare it with unprecedented accuracy to calculated spectra using the same calibrated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

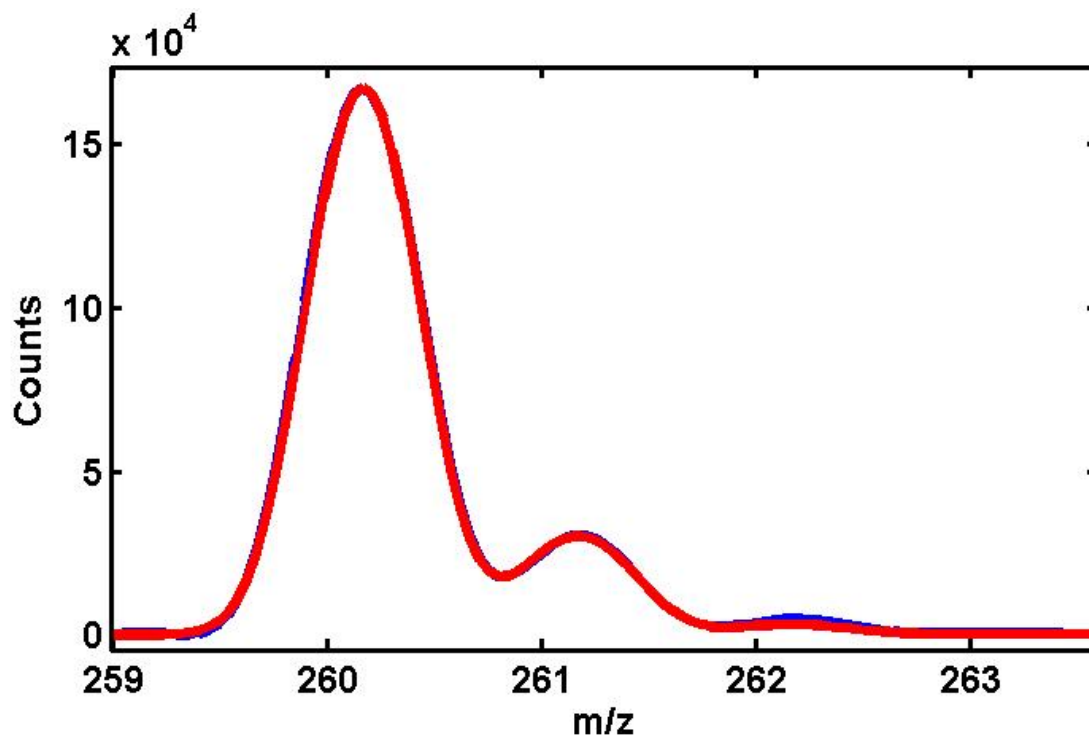


Figure 2 The CLIPS match of the MassWorks calibrated spectrum (Red) against the calculated spectrum of $C_{16}H_{22}NO_2$. The excellent profile match unambiguously identifies this unknown compound.

Target Compound Mass	Calc. Mass	mDa	PPM	Formula	CLIPS Fit %
260.1632	260.1651	-1.9	-7.1	C16H22NO2	0.29
	260.1776	-14.4	-55.5	C17H24O2	0.35
	260.1763	-13.1	-50.3	C15H22N3O	0.37
	260.1525	10.7	41.2	C15H20N2O2	0.41
	260.1637	-0.5	-2	C14H20N4O	0.52
	260.1749	-11.7	-45.1	C13H20N6	0.65
	260.1511	12.1	46.4	C13H18N5O	0.73
	260.1624	0.8	3.2	C12H18N7	0.85
	260.1473	15.9	61.1	C16H22NS	0.94
	260.1599	3.3	12.8	C17H24S	1.01
	260.1439	19.3	74.1	C19H18N	1.03
	260.1498	13.4	51.5	C11H16N8	1.08
	260.1624	0.8	3.2	C13H24O5	1.21

Figure 3 While MassWorks calibration provide excellent mass accuracy, the mass accuracy alone is not sufficient to uniquely identify the target compound (C₁₆H₂₂NO₂). However, the CLIPS isotope profile match uniquely establishes the compound ID (smaller values are better fits).

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 on unknown compounds to assist in their 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 who have access to high resolution systems, it can provide inexpensive and routine ECD on a day to day 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 increase confidence of all measurements.

When is it available?

CLIPS is available commercially as part of Cerno's MassWorks calibration and analysis software starting at version 1.1.

Does it work with other types of instruments/data?

CLIPS also provides greater confidence in ECD measurements for high resolution systems as well. Although high mass accuracy plays a significant role in reducing possible search hits, the mass accuracy alone often can not provide sufficient specificity to effectively determine an unknown molecule even at a very high mass accuracy of 1 ppm. For example, an elemental search for hydroxylated busprione resulted in three different molecular formula, $C_{21}H_{32}N_5O_3$ (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 turn out to be the wrong formula. However, by using CLIPS, the isotope profile enables unambiguous identification of the correct formula.