Introducing...

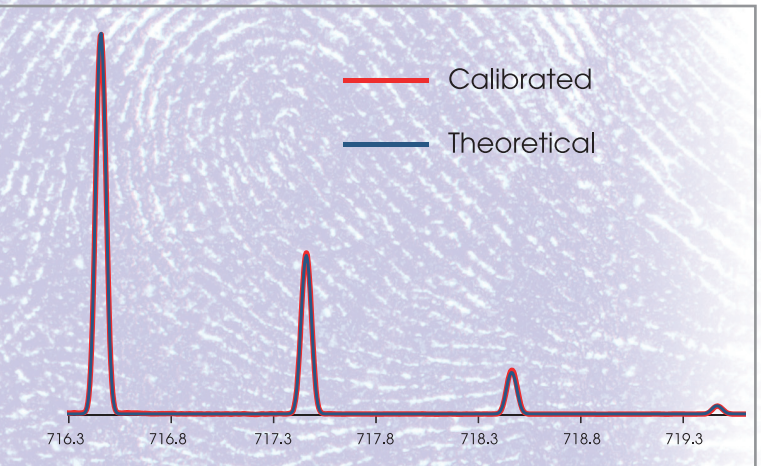
MassWorks™

sCLIPS™

A revolutionary approach for dramatically improving Formula ID from any high resolution Mass Spectrometer

Improved Formula ID from High Resolution MS

- ✓ Line-shape calibration for exact isotope modeling without standards
- ✓ Compare calibrated spectra to theoretical with up to 99.9% Spectral Accuracy
- ✓ Relaxes the need for constant accurate mass [re]calibration
- ✓ For use with all TOF, OrbiTrap, FT-ICR, high res quadrupole, and magnetic sector instruments



sCLIPS™ provides a unique formula ID with FT-ICR MS at 2ppm from over 100 possible formulas

Formula	Mono Isotope	Mass Error (ppm)	Spectral Accuracy
$C_{37}H_{66}NO_{12}$	716.4585	1.68	98.81
$C_{36}H_{63}N_5O_8Na$	716.4574	0.19	98.45
$C_{34}H_{58}N_{11}O_6$	716.4572	-0.20	98.03
$C_{35}H_{54}N_{15}O_2$	716.4585	1.66	97.71
$C_{33}H_{55}N_{15}O_2Na$	716.4561	-1.69	97.41
$C_{35}H_{67}NO_{12}Na$	716.4561	-1.68	97.06
$C_{26}H_{55}N_{21}SNa$	716.4568	-0.74	95.14

••• Over 100 formulas with C, H, N, O, S, Na at 2ppm

sCLIPS (self Calibrated Line-shape Isotope Profile Search) is an entirely new, patented method of MS calibration which can dramatically improve your confidence in mass spec formula ID results from any high resolution instrument. Even with the unparalleled resolving power of FT-ICR-MS reaching as high as 1,000,000, and its highly accurate mass measurement capability with sub-ppm mass error, unique formula determination is rarely possible for true unknowns. This is especially true for ions with m/z values larger than 400Da. For example, even 1 ppm mass accuracy makes you choose from 569 possible formulas for an ion at 477.2303 Da with common organic elements C, H, N, O, S, Cl, P, F, and Na. While the use of the isotope distribution does provide additional useful information, it proves to be quite a challenge to reliably measure the typically small (less than 1%) difference in isotope distribution so as to differentiate among similar formula candidates.

Accurate mass measurements provide you with a choice from a few dozen to hundreds of formula, even at 1ppm mass accuracy. - Spectral Accuracy can tell you which one of the hundreds of formula is the correct one.

MassWorks sCLIPS elegantly addresses this problem by calibrating the mass spec 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. sCLIPS takes advantage of the fact that the monoisotopic peak of an unknown ion is well separated from the rest of the isotopes, providing a direct measurement of the peak shape function, without the use of either internal or external standards. The monoisotopic peak is used by MassWorks to generate a line-shape calibration which is then applied to the ion's entire isotope profile. This line-shape calibrated spectrum can be visually and quantitatively compared to theoretical spectra computed using the very same line-shape function. The resulting Spectral Accuracy value provides an accurate and spectrally interpretable metric to uniquely identify the correct formula from the potentially long list of formula candidates obtained from mass accuracy alone.

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HOW DO I APPLY sCLIPS TO MY DATA?

Performing an sCLIPS search is quick and simple.

- Simply acquire the data using your current MS data system and either directly read native data from major MS vendors into MassWorks or imports ASCII data from your current software via cut and paste or exported ASCII files.
- Click on the monoisotpic peak of the unknown ion and select “sCLIPS” from the drop down menu.
- Set your elements to search, the mass tolerance and click “Search”

That’s it! Within seconds the line-shape calibration is performed, the formula list based on the mass tolerance is created, searched, and sorted by Spectral Accuracy and then displayed in a fully sortable sCLIPS report. You can also inspect various formula candidates by graphically exploring the Spectral Accuracy variations. The reports can be printed or exported via the Windows clipboard.

WHAT OTHER BENEFITS CAN sCLIPS PROVIDE

sCLIPS is quick and easy to perform and requires no calibrants to be measured as the unknown compound provides for a nearly ideal line-shape calibrant. This relaxes the need to perform the sometimes tedious and time consuming protocols to obtain accurate mass measurements. This will save you time and increase your sample throughput, while improving your results as well.

Spectral Accuracy and the ability to compare and overlay the theoretical spectrum can help you easily identify the presence of interferences or improper instrument conditions that can lead to expensive, time-consuming, embarrassing and sometimes dangerous formula mis-identification. sCLIPS can also perform accurate formula ID in the presence of either known interferences or common fragmentation interference such as coexisting M-H, M, or M+H using the powerful mixture search feature. These are capabilities not possible with accurate mass measurements alone.

Formula	Mono Isotope	Mass Error (mDa)	Mass Error (ppm)	Spectral Accuracy
$C_{29}H_{41}N_2O_4$	481.3066	4.93	10.25	99.25
$C_{30}H_{41}O_5$	481.2954	-6.30	-13.09	98.91
$C_{25}H_{37}N_8O_2$	481.3039	2.25	4.67	98.16
$C_{30}H_{37}N_6$	481.3080	6.27	13.03	97.31
$C_{31}H_{37}N_4O$	481.2967	-4.96	-10.31	96.97
$C_{24}H_{41}N_4O_6$	481.3026	0.91	1.89	96.28
$C_{28}H_{41}N_4OS$	481.3001	-1.59	-3.31	96.02
$C_{21}H_{33}N_{14}$	481.3013	-0.44	-0.91	95.94
$C_{27}H_{45}O_5S$	481.2988	-2.93	-6.09	95.73
$C_{23}H_{41}N_6O_3S$	481.2961	-5.62	-11.67	95.38
$C_{22}H_{41}N_8O_2S$	481.3073	5.62	11.67	95.29
$C_{23}H_{45}O_{10}$	481.3013	-0.43	-0.89	94.18
$C_{20}H_{37}N_{10}O_4$	481.2999	-1.78	-3.69	94.06
$C_{18}H_{37}N_{14}S$	481.3046	2.93	6.09	93.84

Table1 The search results for Emetine ($C_{29}H_{41}N_2O_4^+$) sorted by Spectral Accuracy from a TOF instrument. Note the correct formula provides the best Spectral Accuracy. This demonstrates MassWorks sCLIPS can easily discriminate differences as small as a few tenths of a percent, a feat not possible without proper line-shape calibration. Also note that despite the fact the instrument was not well calibrated for mass accuracy, Spectral Accuracy could easily identify the correct compound with a mass error of over 10ppm, which results in 179 formulas using only C, H, N, O and S as the search elements.

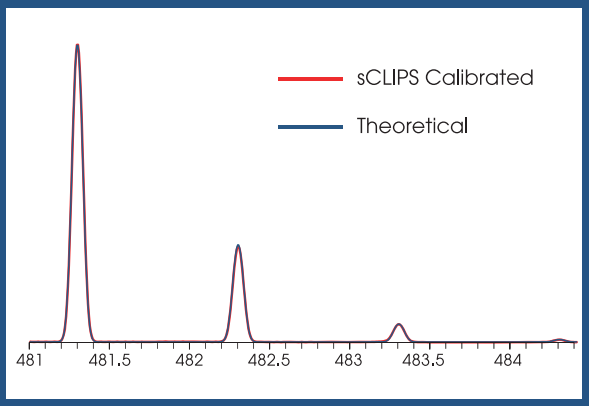

Figure 1 • sCLIPS results for Emetine showing the sCLIPS calibrated spectrum overlaid with the theoretical spectrum for the correct compound.

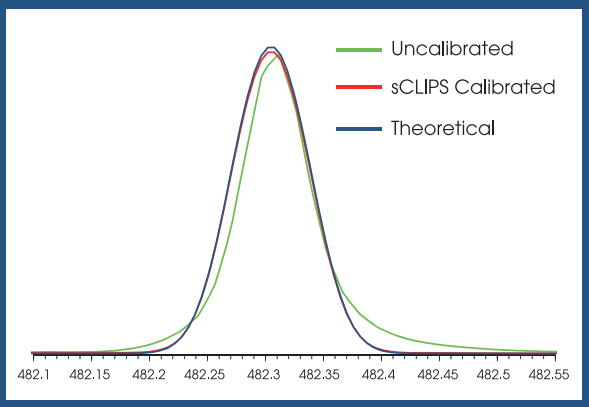

Figure 2 • Zoom in view for the M+1 peak of Emetine demonstrating the large spectral error from the uncalibrated spectrum and the high Spectral Accuracy from the calibrated spectrum.

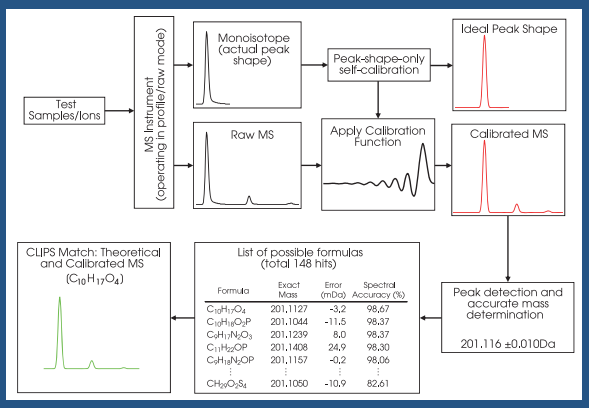

Figure 3 • Flow diagram depicting the sCLIPS calibration and formula determination process. The entire process is automated into a single operation in the MassWorks software.

FOR MORE INFORMATION
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