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MassWorks New Version 7.0

Research Software for Unknown Formula ID. Achieve High Mass Accuracy and High Spectral Accuracy.

Adding to the legacy established in previous versions, MassWorks™ 7.0 is the easy-to-use post acquisition software package that utilizes Cerno's patented TrueCal™ technology to achieve high mass accuracy and high Spectral Accuracy and enable elemental composition determination on conventional mass spectrometers of unit mass resolution using the patented CLIPS™ formula search. MassWorks sCLIPS™ and BestScan™ sCLIPS now also provide high Spectral Accuracy through exact line-shape calibration without the need for standards.

MassWorks integrates the powerful TrueCal calibration technology to obtain up to 100X improvement in mass accuracy on unit resolution systems and up to 99.9% Spectral Accuracy on both high and unit resolution systems in a fast and versatile MS application software package. By combining mass accuracy with Spectral Accuracy, Cerno methodologies can provide significant improvements to all types of MS data, both high and low resolution.

CLIPS search enables unit resolution GC and LC/MS instruments to provide accurate mass formula search

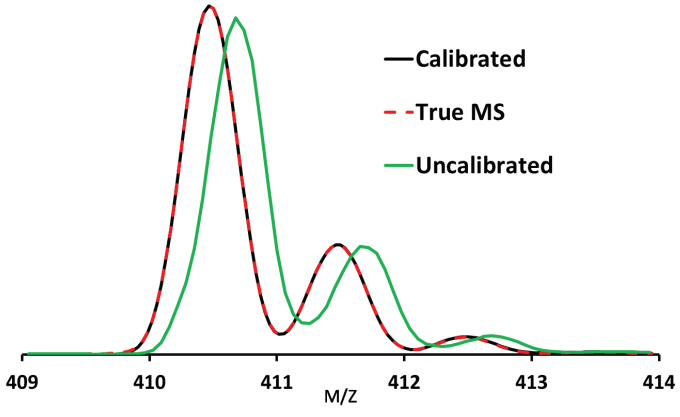
CLIPS (Calibrated Line-shape Isotope Profile Search) combines unsurpassed mass accuracy with the highest Spectral Accuracy to get the most out of your quadrupole MS.

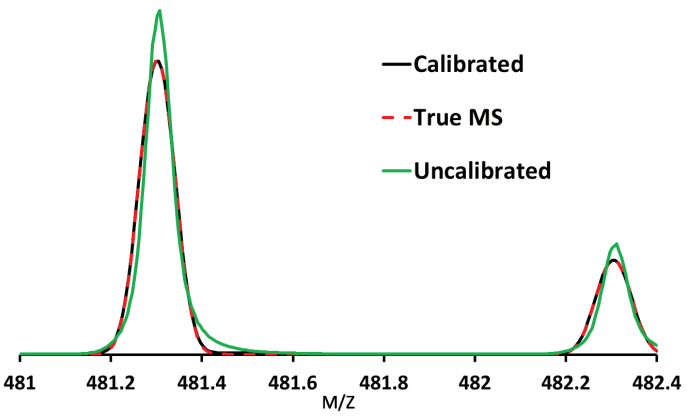
- 100x improvement in mass accuracy from 0.x to 0.00x Da
- Greater than 99% Spectral Accuracy achievable on a chromatographic time scale
- Accurate formula ID enabled even at the unit resolution price
- Powerful mixture analysis of un-resolved MS signals

sCLIPS search for high-resolution MS requires no calibration compounds and dramatically improves Spectral Accuracy for unsurpassed formula ID

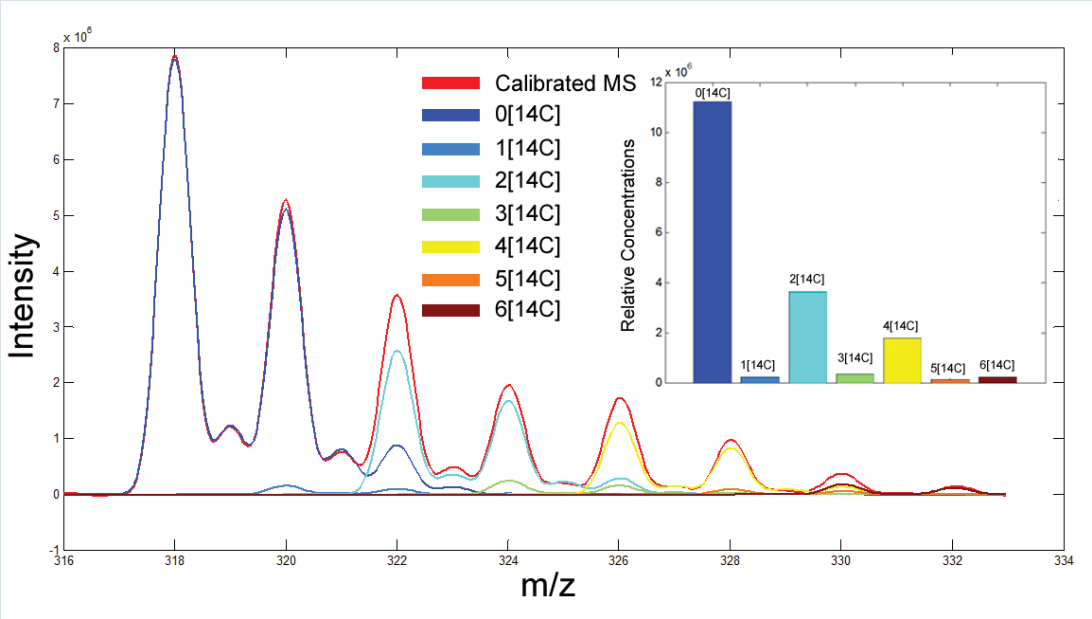
sCLIPS (self-Calibrated Line-shape Isotope Profile Search) allows you to get most from your high resolution TOF, Orbitrap, or FT-ICR.

- Unique, patented self-calibration process
- Mathematically exact isotope modeling
- ≥ 99% Spectral Accuracy achievable on well designed and operated systems
- Going beyond mass accuracy for formula ID
- Capable of eliminating up to 95-99% of incorrect formulas
- Powerful mixture analysis with un-resolved MS signals





Quantitative analysis of complex mixtures of labeled isotopes, biological modifications, and unresolved ions from high and low resolution MS.



TrueCal calibration on both high and low resolution instruments enables powerful quantitative mixture deconvolution never before possible on any MS by utilizing the patented TrueFit™ technology.

The graph illustrates the accurate quantitative analysis of a drug compound containing a [14C] radio-labeled aromatic ring with up to 6 substitutions.

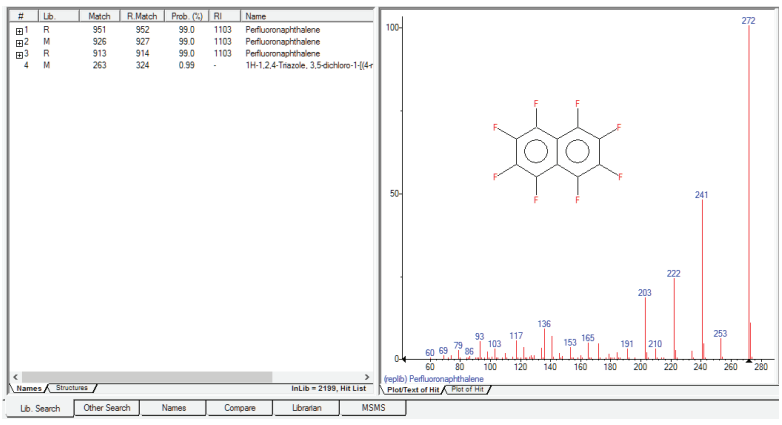
New for MassWorks Version 7

MassWorks Version 7 is now a 64bit Windows application for faster execution and better stability. In addition to the updated file readers, which allows MassWorks to directly read most vendor data, the industry standard NetCDF exchange format is now supported. Also, among the many new features is the addition of "MassLab™" Apps. These custom "Apps" can be created in Python or Matlab to add new capabilities to MassWorks such the exciting new SAMMI™ for large molecule characterization. SAAMI can provide up to 30 times more precision than conventional algorithms on quadrupoles which approaches the accuracy of high resolution instruments.

NIST Library Search integration allows accurate mass search with NIST libraries on low resolution GC/MS systems

GC/MS Library search is a powerful tool for unknown compound identification due to the characteristic fingerprint of the EI fragments. Unfortunately, many hits can be close in match quality and the correct match may be difficult to determine with confidence. Combining the accurate mass search filter with the NIST search reduces the hit list size and improves the confidence in the results. Finally, using the MassWorks CLIPS formula search in combination with NIST search further improves the search confidence. Perhaps most importantly, unresolved peaks can be flagged using Spectral Accuracy, a common problem in GC/MS search.

Each formula listed in the search results is also now directly searchable in ChemSpider as well as the NIST library.



The NIST search shown above illustrates the power of accurate mass library search which filters out many of the incorrect candidates from the NIST search resulting in a much shorter and concise list.

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For More Information

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