

# MassWorks™ v6.0

Novel Software for MS Calibration, Formula ID and Accurate Ion Mixture Quantitation

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BIOSCIENCE

## Solution for Both Unit Mass Resolution and High Resolution Mass Spectrometers

Whether you use a unit mass resolution quadrupole system for GC/MS or LC/MS or any high resolution system such as TOF, Orbitrap, or FT ICR MS, the award winning MassWorks software enables accurate mass elemental composition determination at unit mass resolution while significantly enhancing formula determination capability at high resolution. Details of this innovative MS calibration and analysis technology have been published in a cover feature article in *Anal. Chem.* **2010**, 82, 7055-7062. Operating as an easy-to-use post acquisition standalone software package, MassWorks can read an increasing list of native data from major MS vendors via DirectRead™ including three high resolution MS, MS/MS, and nearly all single quad MS systems. In addition, it retains the capability to import ASCII data from any MS software or data system via cut and paste or exported ASCII files, allowing it to work with virtually any make or model of mass spectrometers. With v6.0, MassWorks continues a capability of relative quantitation of ion mixtures composed of up to **five** additional distinct ion series, arising from low level deamidation or deamination impurities in biologics, overlapping ions from hydrogen-deuterium exchange experiments (HDX MS), ions with multiple / different isotope labels (metabolic flux analysis), ions with their various fragments, and now monomer with its multiply charged multimers.

## Key Features Included in MassWorks v6.0 Premium Software

- *Spectral Accuracy: A measure of the spectral congruency between the MassWorks calibrated profile mode MS data and the true mass spectrum calculated for a given candidate formula (TrueMS™), available inside CLIPS™ and sCLIPS™ as an interactive graphical tool for formula determination*
- *CLIPS™: For quadrupole LC/MS or GC/MS, perform accurate formula ID on these otherwise conventional MS systems with up to 100x better mass accuracy; for linear ion traps, perform formula ID on these conventional MS systems with 10x or better mass accuracy*
- *sCLIPS™: For high resolution MS, such as TOF, Orbitrap, FT ICR, or magnetic sector instruments, dramatically improve the ability to uniquely identify unknown formula by eliminating 95% or more incorrect formula candidates obtained through mass accuracy alone, without the need for calibration standards*
- *Best Scan sCLIPS™: Elemental composition determination by automatically selecting the best ultra-high-resolution MS scan across a chromatographic peak and analyzing the spectrally resolved fine isotopes*
- *High resolution DirectRead support: Agilent TOF/qTOF, Thermo Fisher Orbitrap or FT ICR MS, and Waters TOF/qTOF*
- *AutoCal™: A fully automated accurate mass calibration process for Agilent ChemStation GC/MSD*
- *Unit mass resolution DirectRead support: Advion CMS, Agilent ChemStation/MassHunter/OpenLAB CDS, PerkinElmer TurboMass, Sciex Analyst, Shimadzu LabSolutions LCMS/GCMSsolution, Thermo Fisher Chromeleon/Xcalibur, Waters MassLynx, and Varian MS Workstation*
- *Elemental composition determination/confirmation even in the absence of observable monoisotopic peak signal*
- *Mixture analysis: Accurately accounting for and quantifying up to **five** additional or interfering ion series, each of which may contain more than a dozen ions created by the same repeating unit, available inside CLIPS and sCLIPS for relative quantitation of biologics modifications, labelled isotopes, ion fragments, and monomer/multimers.*
- *Fully integrated accurate mass library search with NIST formatted libraries and online ChemSpider search*

## MassWorks Premium Maintenance Plan

- *Updates and upgrades automatically shipped to the user throughout the period*
- *Unlimited technical support via on-site visits where feasible, WebEx, phone, email or fax*
- *Good for one year starting from the shipment date*

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