MassWorks™ v5.0

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

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 processing 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 major high resolution MS and Shimadzu GC/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 v5.0, MassWorks is now capable 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), and ions with their various fragments.

Key Features Included in MassWorks v5.0 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, 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 removing 95% or more of possible formula candidates obtained by 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 fine isotopes available***
- ***High resolution DirectRead support: Thermo Orbitrap or FT ICR MS, Agilent TOF/qTOF, and Waters TOF/qTOF***
- ***AutoCal™: A fully automated single-step accurate mass calibration process for ChemStation GC/MSD***
- ***Unit mass resolution DirectRead support: Agilent ChemStation, Agilent MassHunter, Thermo Xcalibur, Waters MassLynx, Varian MS Workstation, Shimadzu LabSolutions LCMS, Shimadzu GC/MS, PerkinElmer TurboMass, Sciex Analyst, and Advion CMS***
- ***Elemental composition determination/confirmation even in the absence of observable monoisotopic peak***
- ***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 (including Best Scan sCLIPS) for relative quantitation of biologics modifications, isotope labels, or ion fragments***
- ***Fully integrated accurate mass library search with NIST GC/MS EI library 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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