Agilent MassHunter Workstation Software

A faster, more confident path to all the information in your samples.

Our measure is your success.

products | applications | **software** | services

Agilent Technologies

Are you looking for peaks and data points? Or are you looking for answers?

From instrument tuning to final report, Agilent's MassHunter Workstation software is designed to make all your MS analyses faster, easier and more productive.

The software provides a single acquisition platform for Agilent LC/MS TOF, Q-TOF and triple quad instruments—and a single, consistent data processing package for all of your Agilent MS platforms, including LC/MS, GC/MS and ICP-MS.* In addition, it incorporates advanced feature extraction, data mining and data processing tools that let you rapidly and accurately extract all available information from the compounds in your samples. Not just peaks and data points, but answers.

***MassHunter Workstation** software's powerful feature extraction and data mining capabilities perfectly complement the best-in-class performance of Agilent's LC/MS, GC/MS and ICP-MS platforms.**

MassHunter's fully automated data analysis routines fully exploit the high information content of accurate-mass MS and MS/MS data from Agilent TOF and Q-TOF LC/MS systems. So you can:

- **Confidently find all compounds in your samples or differences between samples and sample sets.** MassHunter software helps you extract all relevant information in a chromatographic run—not just chromatograms and spectra.
- **Easily confirm and identify unknowns.** MassHunter software simplifies data mining and automatic identification by using the accurate-mass optional retention time (AMRT) database, MS/MS library searches (coming soon) and molecular formula generation (MFG).

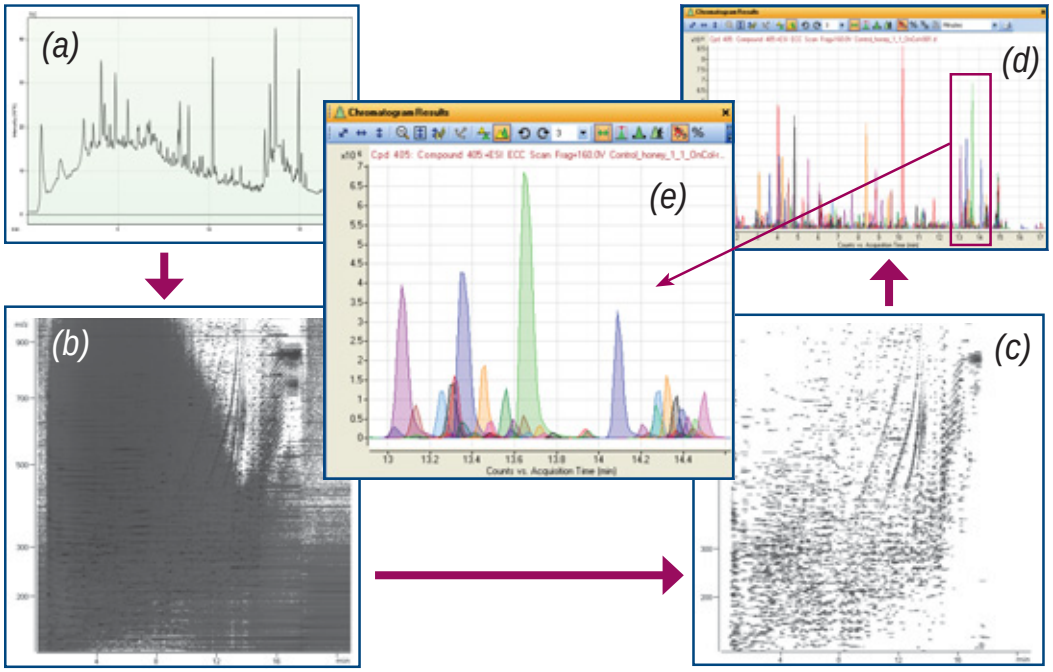
**MassHunter Workstation for GC/MS and LC/MS single quad is coming soon.*

Unprecedented data processing productivity

"Compound-centric" data processing and intuitive, workflow-driven navigation shorten the path between raw analytical results and the answers you're looking for. So you can:

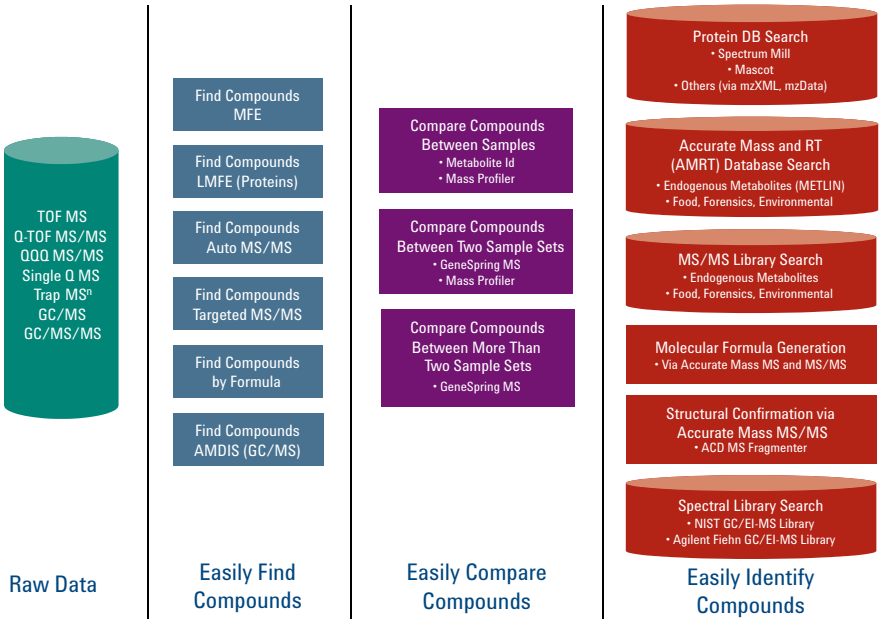
- **Spend less time with quantitative analysis.** A powerful, application-centric quantitation package with task-driven functionality eliminates tedious manual processing steps.
- **Review results of complex data, quickly and easily.** An innovative user interface displays all relevant info at a glance and lets you easily compare data files.
- **Minimize analysis time and maximize your lab's throughput.** Timesaving features such as a curve-fit assistant, dynamically linked results, outlier flagging, batch-at-a-glance data review and customizable views help to speed up every analysis.

More thorough analysis, more confident results



Powerful tools help you extract the information you're looking for. *Unlike traditional data processing software that works on 2D chromatograms (a), MassHunter Workstation software uses its unique Molecular Feature Extractor (MFE) algorithm to work directly with the 3D accurate mass LC/MS data set (b), MFE fully and automatically removes noise due to matrix contribution (c) and extracts compound chromatograms (d) and compound mass spectra for each component. The overlaid compound chromatograms (e) show the exact location and elution profile for each compound in the sample, even if multiple compounds partially or fully co-elute.*

Compound-centric approach integrates seamlessly with your workflows

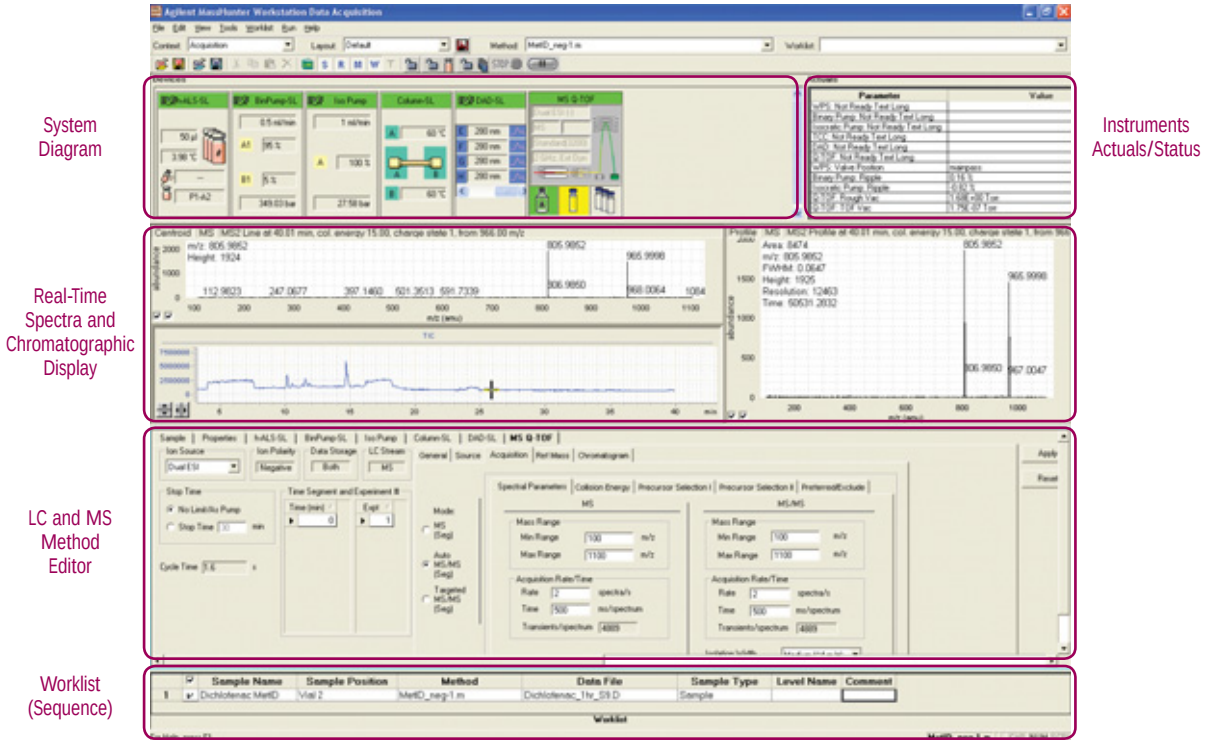


Agilent MassHunter software is designed around your workflows. *One easy-to-learn interface not only handles your basic qualitative and quantitative analysis tasks, but also integrates seamlessly with applications such as Metabolite ID, Metabolomic Profiling, Biomarker Discovery and Intact Protein and synthetic peptide characterization. (See page 7, "Integrated, application-driven database and library searching.")*

To learn more about Agilent MassHunter Workstation software, visit www.agilent.com / chem / masshunter

All the relevant information, at your command.

MassHunter Workstation's intuitive, "flat" user interface lets you see all relevant information at a glance. You don't have to switch views or dodge annoying pop-up boxes to find what you're looking for. The workflow-driven layout even minimizes mouse travel and the number of clicks you need. The software also provides full support for dual monitors.



Instrument set-up and control. *On a single screen, MassHunter Workstation's Data Acquisition software gives you everything you need to monitor and control your run.*

One acquisition software for all LC/MS platforms

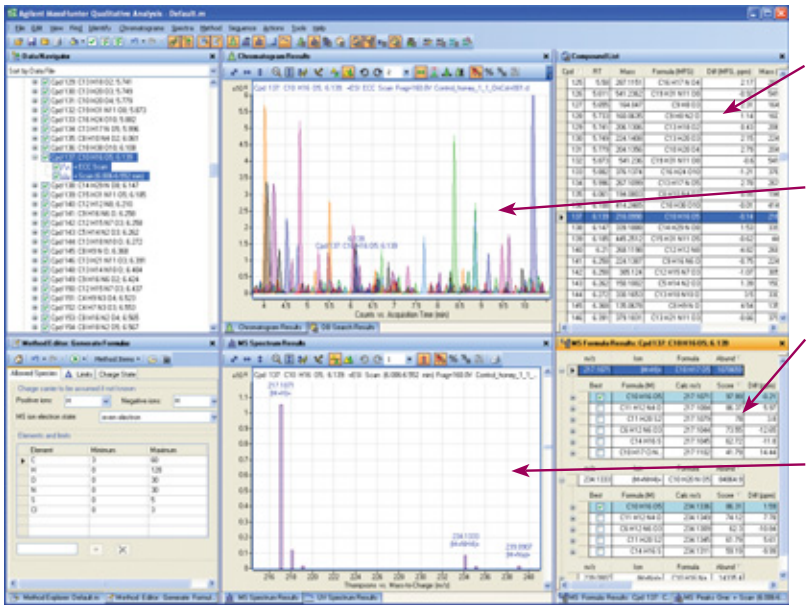
The MassHunter acquisition software features comprehensive data-dependent and targeted MS/MS capabilities for the Q-TOF, as well as automated MRM method development software (MassHunter Optimizer), scheduled MRM and 21CFRPart11 compliance support for the triple quad instrument. All instruments share the control of LC modules and a worklist editor, with features similar to Microsoft Excel® spreadsheet software, to set up the acquisition of multiple samples.

Innovative compound-centric data navigation

Compound-centric data organization and navigation make it easy to review and analyze complex MS data. In MassHunter Qualitative Analysis, all automatically extracted spectra and chromatograms are organized as entries in a navigation tree and can be navigated compound by compound.

The entries are dynamically linked with compound mass spectra and chromatograms, mass lists and a configurable table summarizing all compound-specific results that could be extracted. Results can also include information from additional processing steps such as molecular formula generation, charge state assignment and deconvolution, AMRT database search results, Find-by-Formula results and MS/MS library search* results.

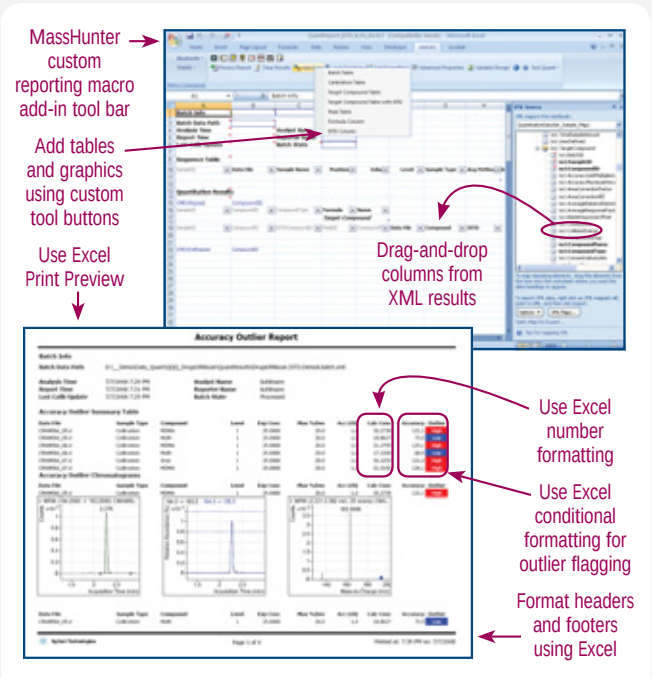
**MS/MS libraries coming soon.*



Qualitative Analysis. *MassHunter Workstation's workflow-based user interface enables fast, intuitive compound-centric data mining and navigation, and shows you the information you need at a glance.*

Compound-centric results storage and reporting, too

MassHunter Workstation software stores all processing results on a compound-by-compound basis along with the data file, including compound spectra, compound chromatograms, molecular formulas, database and library search results, charge state, deconvolution results, isotope pattern, and more. You can report results on a per-compound basis using MassHunter's highly customizable reporting based on Microsoft Excel® spreadsheet software and XML results files.



Fully customizable reports enable collaborative, better-informed decision making

Presenting critical information from your MS experiments helps your organization make important scientific or business decisions. MassHunter stores all results in XML files and uses Microsoft Excel and a custom macro add-in for reporting. A wide range of application-specific report templates or customized reports is available in this familiar Excel environment, including custom calculations to meet your needs.

Archive MassHunter data, results and methods in Agilent OL ECM

For archiving MassHunter data files, including results and methods, a seamless integration with Agilent OpenLAB Enterprise Content Manager (ECM) enables easy indexing and searching of all sample information with automatic scheduling of data transfer to an ECM server.

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Powerful tools help you extract the information you're looking for.

With MassHunter Workstation software, you can instantly focus on the important questions when reviewing chromatographic and mass spectral results: What is in my sample? How much is there? What is different between these two samples? How do these sample sets compare?

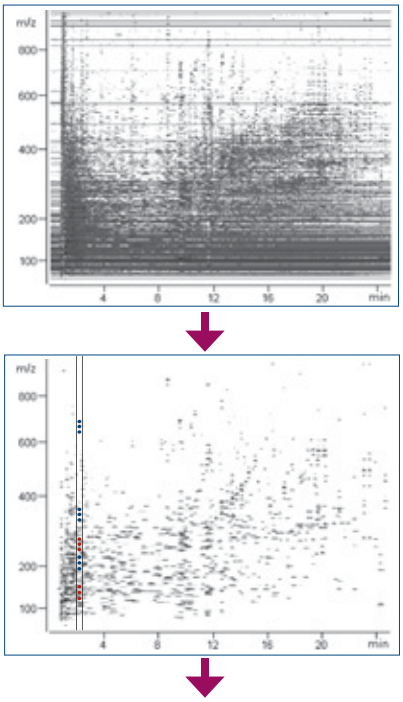
MassHunter software fully taps into the information potential of accurate-mass MS and MS/MS data. Proprietary algorithms enable comprehensive data mining to bring the highest level of certainty to confirmation and identification of unknowns. If it's there, MassHunter will help you find, identify and quantitate it.

Molecular Feature Extractor streamlines ID and profiling studies

The advanced Molecular Feature Extraction (MFE) algorithm built into MassHunter software saves hours of analysis time by automatically locating all sample components down to the lowest level abundance and extracting all relevant spectral and chromatographic information. The software can also execute additional processing steps, such as molecular formula generation, AMRT database or MS/MS library search,* deconvolution or charge state determination.

A tremendously powerful and useful capability, MFE has three general uses:

- For **qualitative analysis,** MFE finds all detectable compounds—known and unknown—in a single sample.
- In **metabolite ID and similar applications,** MFE finds all compounds in two samples and compares them in order to find compounds of interest that differ significantly between the samples.
- Used in **mass profiling studies**—for example, in biomarker discovery—MFE finds compounds in each of many samples. Results can be imported into Mass Profiler or GeneSpring MS software for statistical analysis to find significant differences between sample sets.



List of compounds or molecular features

RT	m/z	Abund
---	---	---
---	---	---
2.11	195.1745	21000
2.11	257.2566	335500
2.34	224.2134	11784
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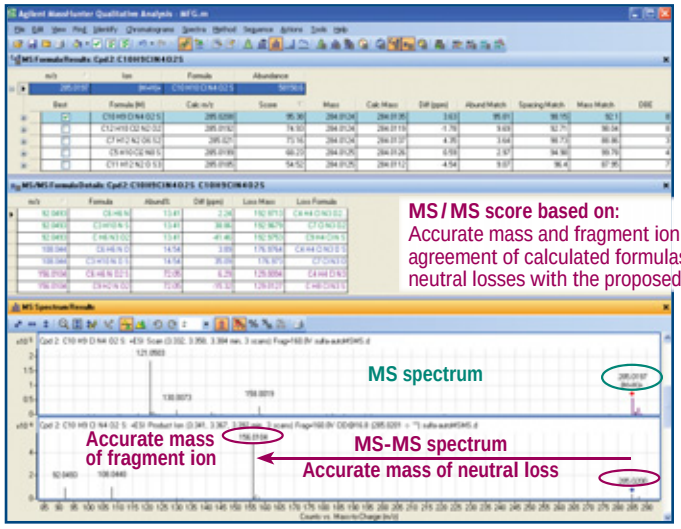
Molecular Feature Extractor *quickly and automatically turns highly complex LC/MS data files into a complete, accurate list of compounds or molecular features with retention time* m/z *and abundance.*

**MS/MS libraries coming soon.*



MS score based on:
- Accurate mass of all compound ions
- Isotope abundance pattern
- Isotope spacing of M+1 and M+2

MS / MS score based on:
Accurate mass and fragment ion coverage, requiring agreement of calculated formulas for fragment ions and neutral losses with the proposed precursor ion formula

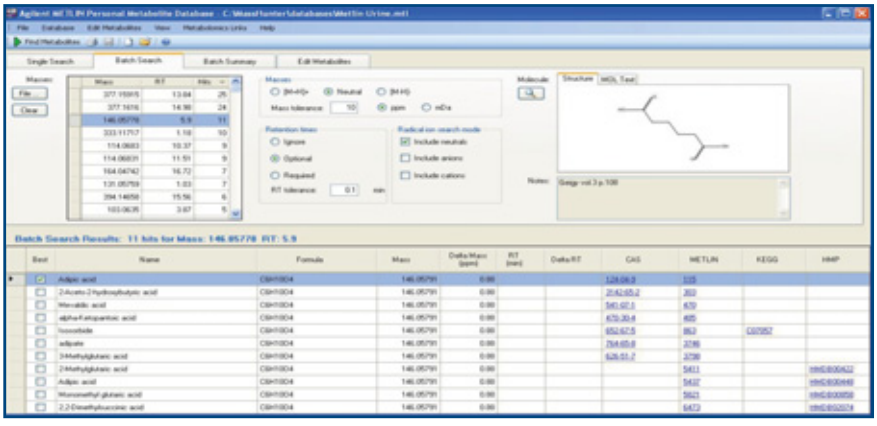
Accurate mass information used:
- From precursor ion
- From isotopes M+1, M+2
- From each fragment ion
- From each neutral loss

Molecular Formula Generator *(MFG) software uses multiple dimensions of information to generate and score lists of possible molecular formulas. The software reduces the number of plausible formulas by using the accurate mass information contained in the MS/MS spectra.*

Integrated, application-driven database and library searching

To enhance your productivity—and to make compound identification easier—MassHunter Workstation software lets you perform automated accurate-mass searches of compounds of interest against METLIN, Spectrum Mill and other public and private databases. Compounds can be identified conducting an AMRT database search, performing an MS/MS library search* or doing a Molecular Formula Generation using accurate mass MS and MS/MS information, in parallel or in sequence.

(Agilent is also developing content databases and MS/MS libraries for food, forensics and environmental applications; coming soon.)



Agilent's METLIN Personal Database. *METLIN is the most complete metabolite database in the world, with more than 22,000 primary and secondary endogenous metabolites, including lipids and di- and tripeptides as well as common exogenous metabolites. With this personal database, your searches remain completely confidential; you can also customize by adding proprietary compounds and/or retention times.*

**MS/MS libraries coming soon.*

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Agilent Mass Profiling Workflow: Discover statistical differences faster and more reliably.

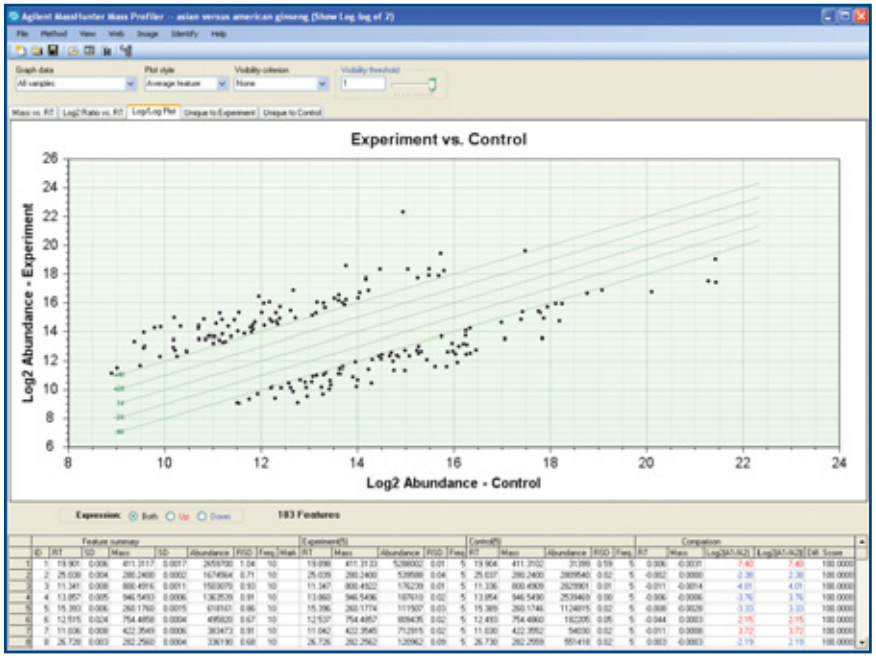
MassHunter Qualitative Analysis, Mass Profiler and GeneSpring MS software are part of Agilent's integrated Mass Profiling workflow—a seamless MS hardware and software solution that streamlines studies where it is necessary to find differences between sample sets.

Originally developed for proteomics and metabolomics studies, the mass profiling workflow also supports additional differential analysis applications such as pharmaceutical impurity testing, forensics, and environmental and pesticide analysis. The unique MFE algorithm lets you confidently locate all the components of interest in an individual sample, even in very complex mixtures.

Every step optimized for comprehensive results and maximum productivity

For challenging expression profiling and biomarker discovery applications, the MassHunter Qualitative Analysis software first simplifies a complex data set of accurate mass MS results. A variety of statistical methods and visualization tools employed by Mass Profiler or GeneSpring MS software allows the identification of meaningful differences between sample groups, e.g., healthy versus diseased population, and the calculation of the abundance ratios of differentially expressed features. Both Mass Profiler and GeneSpring MS allow flexible selection of the comparison criteria and inspection of any selected feature.

The list of differently expressed compounds can then be exported for search in AMRT databases such as METLIN, LC/MS/MS libraries* or the Agilent Fiehn GC/EI-MS library. Identification results can also be exported into pathway analysis software packages.



***Mass Profiler software** includes easy-to-use statistical and visualization tools that allow the identification of statistically meaningful differences between two sample groups.*

**MS/MS libraries coming soon.*

LC/MS
GC/MS

MFE (LC/MS)
AMDIS (GC/MS)

Mass Profiler
GeneSpring MS

Spectrum Mill
Mol. Formula Gen.
AMRT DB Search
Library Search

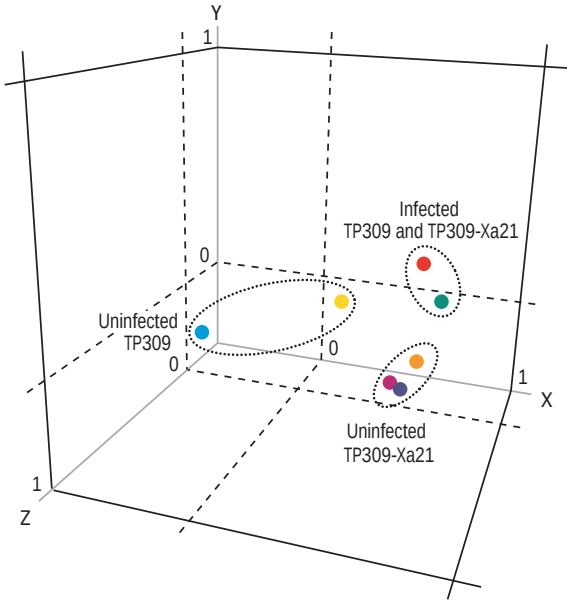
QQQ MRM
GeneSpring MS

Agilent's powerful Mass Profiling workflow involves a number of steps supported by Agilent MS hardware and software tools, including:

1. LC/MS or GC/MS data acquisition.
2. Automatic extraction of compound information via Molecular Feature Extraction or AMDIS, resulting in compound lists with mass, RT and intensity for each compound; compound information is aligned in RT and intensity between each individual sample, based on added internal standards or all contained compounds.
3. Statistical analysis of compound lists to find significant differences between the sample sets, using either MassHunter Mass Profiler for simple differential analysis between two sample sets or GeneSpring MS for sophisticated statistical analysis between two or more sample sets.
4. Identification of compounds that show significant differences in abundance.
5. Where required, validation of potential biomarkers via higher throughput-targeted MRM quantitation (triple quad), or SIM (GC/MS) and statistical analysis in GeneSpring MS.

Agilent GeneSpring MS software helps you elucidate biological relevance

Designed to integrate data and results from multiple applications, as well as other statistical analysis packages, GeneSpring MS lets you easily import, normalize, compare and display GC/MS, LC/MS, and CE/MS data—including MS/MS data—from large sample sets and complex experimental designs.



***GeneSpring MS** is a unified, easy-to-use platform for mass spectral data normalization and comparison that helps you answer the complex biological questions targeted by metabolomics and proteomics studies.*

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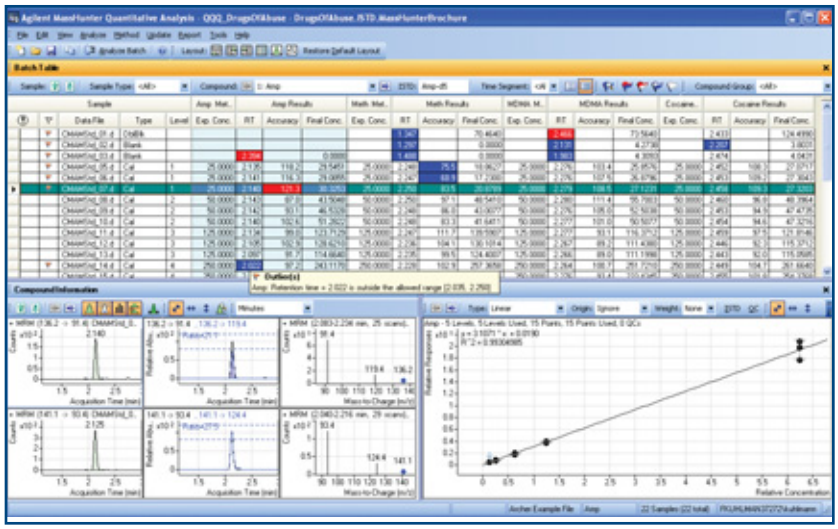
MassHunter Quantitative Analysis Software

Fast, powerful quantitative analysis

Easy to learn and use, MassHunter's Quantitative Analysis software offers unprecedented productivity for large, multi-compound batches. A parameterless integrator with built-in peak validation capability lets you focus on problem peaks only. The software also provides tools for work in 21CFRPart11 compliant environments, including user login, session lock, configurable user roles, electronic signatures and a comprehensive audit trail.

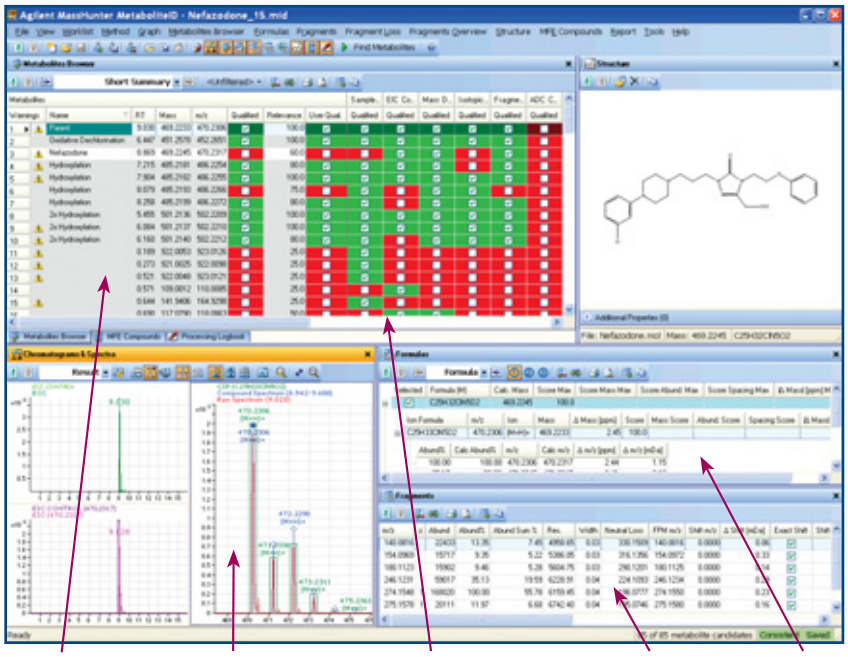


MassHunter Quantitative Analysis Software ensures that you spend less time analyzing your data. *It includes helpful features such as batch-at-a-glance data review, a curve-fit assistant, dynamically linked results, outlier flagging and customizable views. All this, with the flexibility of compound- or sample-centric navigation.*

MassHunter Metabolite ID Software

Comprehensive, confident metabolite identification

With the widest selection of algorithms available in the industry, MassHunter Metabolite ID lets you find and confirm expected metabolites via accurate mass, isotope pattern, MS/MS spectrum, UV peak, radioactivity detector peak and mass defect. You can also identify unexpected metabolites via accurate mass or calculated molecular formula based on MS or MS/MS data.

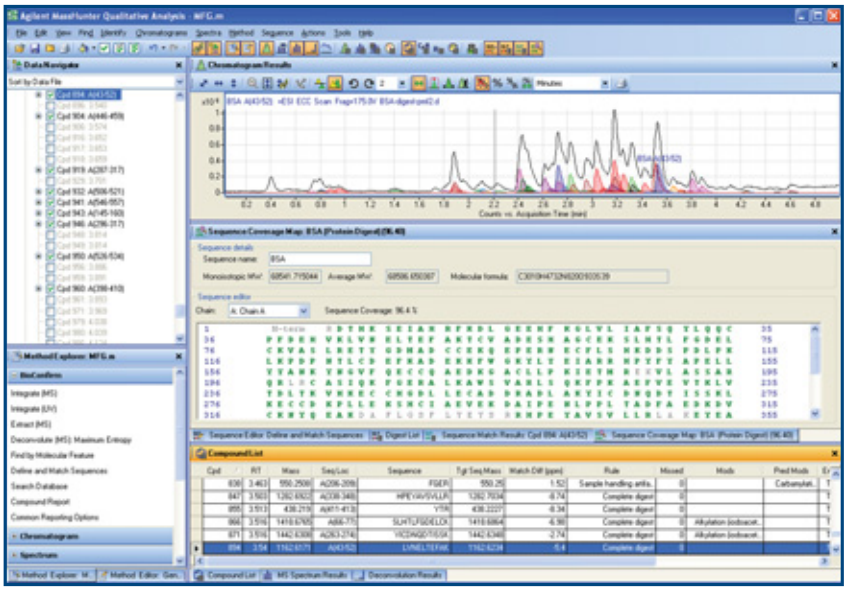


MassHunter Metabolite ID software *simplifies metabolite identification without taking away your choice or control. The versatile, powerful application package can reduce your data processing, review and reporting from days to hours.*

MassHunter BioConfirm Software

Positive confirmation of synthetic peptides and intact proteins

MassHunter BioConfirm software helps you confirm identities of synthetic peptides and identify variants of intact proteins such as antibodies. The software uses sophisticated algorithmic tools for automated, unattended or interactive confirmation and characterization of recombinant proteins or synthetic peptides, providing an accurate determination of the mass and abundance of each peptide or protein variant.

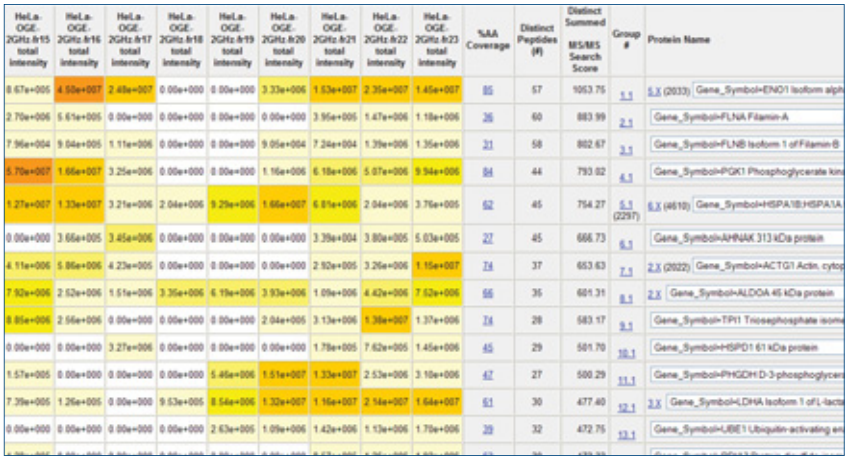


Interactive Sequence Editor / Matcher *in the BioConfirm software helps locate the site of the modification, when analysis of recombinant proteins indicates that the wrong protein was produced. The unique protein Molecule Feature Extractor enables complex mixture analysis via related ion deconvolution.*

Spectrum Mill for MassHunter Workstation

Rapid protein identification and quantitation

Spectrum Mill for MassHunter Workstation quickly identifies proteins and peptides via fast database searches and provides automatic and manual match validation. It also offers *de novo* sequencing of peptides not found in any database. Proteins of interest can be quantified by comparing relative abundances of all component peptides observed for a given protein, using either isotope-labeling or label-free strategies with superior visualization tools. Peptide Selector Tool predicts optimal peptides and MS/MS product ions for targeted quantitative proteomics.



Spectrum Mill for MassHunter Workstation *accurately determines not only protein identities but also relative abundances of a given protein in multiple samples. Color coding makes relative abundances apparent at a glance.*

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Make all your MS analyses faster, easier and more productive

From instrument tuning to final report, Agilent MassHunter Workstation software's advanced control and data analysis capabilities are the perfect complement to the power and performance of your Agilent mass spectrometry systems.

For more information

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U.S. and Canada
1-800-227-9770
agilent_inquiries@agilent.com

Europe
info_agilent@agilent.com

Asia Pacific
adinquiry_aplsca@agilent.com

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