

Agilent MassHunter Software

YOUR FASTER ROUTE TO INSIGHT

The Measure of Confidence



Agilent Technologies

MASS SPECTROMETRY AND THE DATA CHALLENGE

Mass spectrometry continues to provide more comprehensive data than we ever imagined possible, enabling us to detect and identify analytes orders of magnitude lower than just five years ago. With this abundance of data comes additional challenges related to fast interpretation to achieve actionable results.

Scientists often struggle with:

- Large data sets that reduce throughput
- High training costs for multiple software platforms across the lab
- Manual review of the data—requiring significant time and introducing inconsistencies
- Dealing with the complexities of exporting and cross referencing data with other programs.

Agilent MassHunter software is designed to make your MS analyses faster, easier, and more productive. In addition to data acquisition and instrument control for your Agilent LC/MS, GC/MS, CE/MS, and ICP-MS, the software incorporates advanced data mining and processing tools. These let you rapidly and accurately extract all available information from the analytes in your samples—not just peaks and data points, but answers.

"The software is very, very user-friendly. Step-by-step, I learned quite easily on my own. So many possibilities to give meaning to my data. And all of them are efficient and powerful, and help me to get some nice conclusions on the hypotheses I have made at the outset."

DR. LUIGI LUCINI, LC/MS USER, INSTITUTE OF ENVIRONMENTAL AND AGRICULTURAL CHEMISTRY AND RESEARCH, CENTRE FOR PROTEOMICS AND NUTRIGENOMICS, UNIVERSITY CATTOLICA DEL SACRO CUORE

See MassHunter in action online. Experts demonstrate the capabilities of various MassHunter features at www.agilent.com/chem/masshunter

"At the American games in Mexico, having an option like Compounds-at-a-Glance made it very easy to detect which compounds are positive. Also, having the capability to customize our reporting is very important because we are continuously adding new compounds to the methods and we need to incorporate them into the reporting template."

DR. JOSEP MARCOS, LC/MS USER THE HOSPITAL DEL MAR IN BARCELONA

"I see software as a tool for me to get to my really exciting stuff, the biology. MassHunter is really good—it's developed over time and it's gotten better and better. It also interacts really well with some of the non-proprietary software we use. With MassHunter, we don't suffer the frustration of delayed results that we do with some other software packages."

DR. NICOLAS TAYLOR, LC/MS USER, MOLECULAR ACCLIMATION LABORATORY, ARC CENTRE OF EXCELLENCE IN PLANT ENERGY BIOLOGY, UNIVERSITY OF WESTERN AUSTRALIA

A SINGLE, CONSISTENT USER EXPERIENCE ACROSS ALL YOUR AGILENT MS PLATFORMS

One easy-to-learn software platform handles all your qualitative and quantitative analysis tasks. Because common data analysis tools are shared from one Agilent MS platform to the next, you will reduce training time, minimize operator errors—and significantly increase your lab's productivity.

Comprehensive software for LC/MS, GC/MS, CE/MS, and ICP-MS workflows

MassHunter uses dedicated software modules for instrument-specific tasks including identification, characterization, quantitation, target analyte screening and confirmation, unknown identification, characterization of biomolecules, nanoparticles, elemental species, and protein and metabolite identification. This comprehensive suite of software programs creates seamless workflows for

your application from sample submission to reporting. With hyphenated systems composed of multiple Agilent instruments such as LC- or GC-ICP-MS, MassHunter integrates the software components into a single tool for the specific task.

Customizable to your workflow

Agilent MassHunter enables analyzing hundreds of thousands of compounds or thousands of samples per day. Powerful modules let you to integrate new features that support specific workflow solutions,

such as BioConfirm for biopharmaceuticals, PCDLs for food, environmental, forensics, and pharmaceutical applications, DrugQuant for drug confirmation, and specific solutions for USEPA and USP methods. Mass Profiler Professional, Unknowns Analysis, and characterization and quantitation of nanomaterials also help you extract the maximum information from your samples.

SHORTEN THE PATH TO YOUR RESULTS WITH MASSHUNTER QUANTITATIVE ANALYSIS

MassHunter quantitative tools support you with quick analysis and review

- Time-saving features such as batch-at-a-glance data review, compounds-at-a-glance, dynamically linked results, and customizable views
- Comprehensive features to support quantitation in compliance with US EPA and 21 CFR Part 11 with OpenLAB Enterprise Content Manager (ECM)
- Over 40 integrated quality test criteria, and a parameter-less integrator with built-in peak validation capability that lets you focus exclusively on problem peaks and minimize manual reintegration
- Color-coded outlier detection complements flexible, spreadsheet-like organization of the data for predefined quality tests, drawing your attention to results that require closer inspection.
- Simple, quick creation of quantitative methods with tools such as Concentration Setup Assistant
- Click a result and all associated peaks, spectra, and calibration data are immediately displayed. Additional pop-up information is available.

"One of the great things about MassHunter is that you can walk up to a triple quad to do acquisition, and it's the same software that you walk up to for the Q-TOF and even a GC/MS instrument. That really makes training a lot easier because we haven't got different software for every different instrument."

DR. NICOLAS TAYLOR, LC/MS USER, MOLECULAR ACCLIMATION LABORATORY, ARC CENTRE OF EXCELLENCE IN PLANT ENERGY BIOLOGY, UNIVERSITY OF WESTERN AUSTRALIA

"We work with QC analyses that involves tracking 40 parameters, looking at a sequence of 10 samples at a time... before, we had to go sample by sample, data file by data file to evaluate the sequence... Now, with MassHunter, we have created one customized overview screen that enables us to scroll parameter by parameter all the QCs for the full sequence very quickly."

DR. ARMAND VERBUEKEN, GC/MS USER, BAYER, ANTWERP, BELGIUM ENVIRONMENTAL TESTING LAB

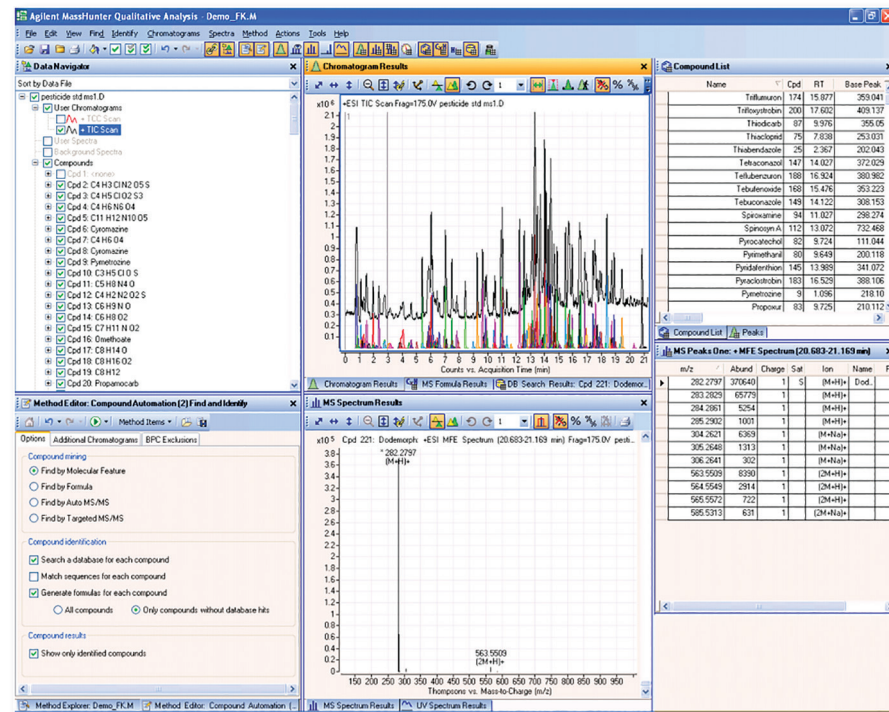
"MassHunter Quantitative Analysis accelerates our time to results. Integrating historic compound-specific performance as set points for the immense number of flagging options in the software provides us a high level of quality control for our assays. The review-by-exception approach with Outliers is helping us to dramatically reduce the time we spend reviewing data without any concerns over loss of quality."

FREDERICK G. STRATHMANN, PHD, DABCC (CC, TC); MEDICAL DIRECTOR OF TOXICOLOGY AND ASSOCIATE SCIENTIFIC DIRECTOR OF MASS SPECTROMETRY, ARUP LABORATORIES, ASSISTANT PROFESSOR, DEPARTMENT OF PATHOLOGY, UNIVERSITY OF UTAH

QUALITATIVE—LC/MS, GC/MS—POWERFUL AND CUSTOMIZABLE

No more missing information

The powerful tools of MassHunter Qualitative Analysis help you extract all the information from your samples. Advanced data mining and processing options, such as Molecular Feature Extractor and integrated deconvolution algorithms, let you rapidly and accurately find all detectable compounds and easily confirm targets or identify unknowns. MassHunter's unique, compound-centric data organization and navigation lets you easily compare complex MS data files, and review results quickly and efficiently.



MassHunter Qualitative Analysis has a compound-centric user interface that allows for quick review of chromatograms and spectra across data files.

BRING NEW POWER TO YOUR LC/MS WORKFLOW

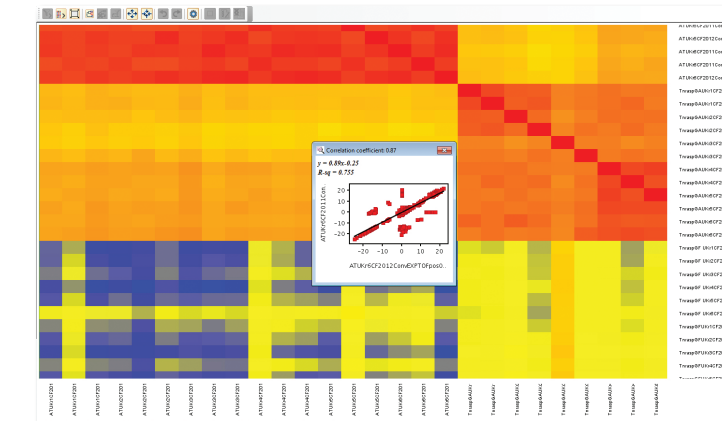
MassHunter Walkup software makes LC/MS accessible to more scientists—for medicinal chemistry, drug discovery, chemistry, and biopharmaceutical labs

Agilent MassHunter Walkup software helps users of different skill levels to perform their own automated LC and LC/MS analyses. All that's required is to input some basic information, choose a method, and place samples as directed. Results show up in the submitter's email in-box automatically.

The software also enables administrators to tailor user access to instrument parameters, significantly reducing the possibility of operational errors that can lead to costly instrument down time. Automatic notifications can be delivered when there is an instrument error.

Mass Profiler Professional lets you easily classify, compare, and analyze sample groups

Agilent Mass Profiler Professional's powerful analytical capabilities fully exploit the high information content of mass spectrometry data.



Agilent Mass Profiler Professional helps you easily detect differences in your data. Brain tumor subgroups were identified using 370 differential proteins with sample-to-sample correlation and Principal Component Analysis.

"Using MassHunter Qualitative, we were able to develop personal data reference standards for selected defects in olive oil. This helps to ensure confident classification of olive oils, and resolve disputes when the sensory assessors conflict."

DR. LANFRANCO CONTE, GC/MS USER, DEPT. OF FOOD SCIENCE, UNIVERSITY OF UDINE, ITALY

"MassHunter Walkup makes our instruments 'easy to use and hard to break'. MassHunter's ease of use helps us bring complex assays done by experts to a Walkup method."

MUHAMMAD ASIF ALIMUDDIN, OPEN ACCESS LAB ADMINISTRATOR, MAJOR PHARMACEUTICAL COMPANY

FAST, INTEGRATED LIBRARY SEARCHES SUPPORT YOUR UNDERSTANDING

To enhance your productivity and more easily identify targeted and untargeted analytes, MassHunter Workstation can automatically search significant compounds against METLIN, the Fiehn Library, NIST, Spectrum Mill, and many other application-focused databases. Best-in-class algorithms, optimized for your MS platform, ensure the highest accuracy.

Market-focused MS and MS/MS libraries for pesticides in food safety and forensics/toxicology provide specific information for your application, for example:

- The Fiehn GC/MS library contains the most comprehensive GC/MS EI library of metabolite spectra
- The METLIN Library contains MS/MS spectra for high confidence identification of thousands of metabolites

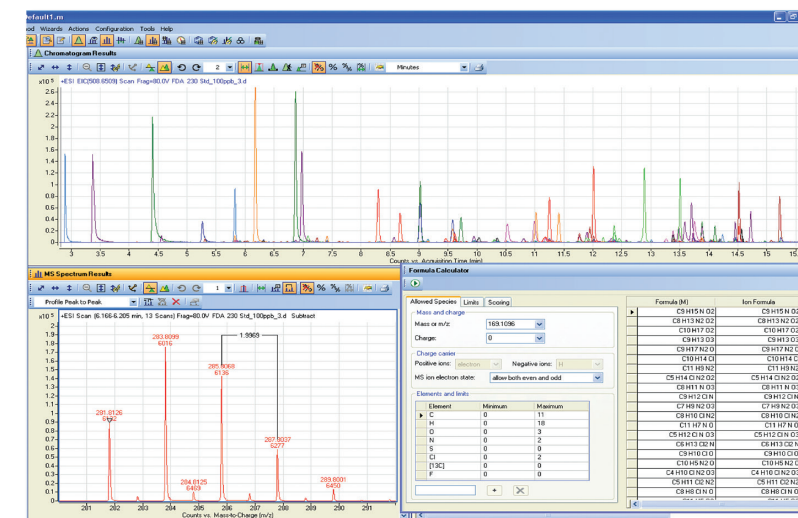
PERSONAL COMPOUND DATABASE AND LIBRARIES ENHANCE TARGETED SCREENING

The Agilent Personal Compound Database and Library (PCDL) is an integral part of our targeted screening workflows that use the All Ions MS/MS technique for LC and GC TOF and Q-TOF. Identification results from databases and libraries can easily be used in other MassHunter programs such as Pathway Architect for pathway analysis.

Agilent is the leader in identification!

Here's a list of the Agilent databases and PCDLs that are currently available. We continually work to develop new databases and enhance our existing databases.

- Pesticides PCDL
- Mycotoxins PCDL
- Veterinary drugs PCDL
- METLIN database



Agilent MassHunter Qualitative Analysis software supports peak finding of GC/MS data files, and compound identification via library matching.

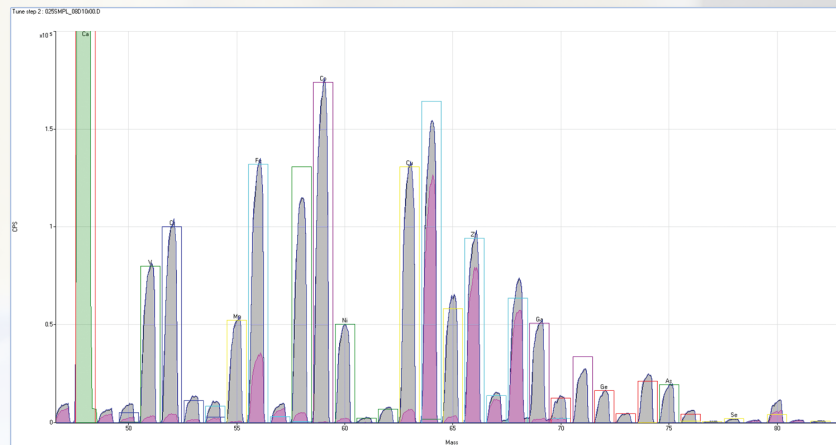
Compound Name	Formula	Mass	Acen	Cation	RT (min)	CAS	ChemSpider	IFPAC Name	Spectra	Notes
Chlorophenol	C ₆ H ₅ ClO	147.0283				107-11-1	107-11-1	2,2-Dichloro-1,1,1-trifluoroethane	6	Forensic and Toxicology; drug; Veterin...
Morphine	C ₁₇ H ₁₉ N	285.3406				59-03-9	59-03-9	3,6-Epiacetylmorphine-3-O-acetate	6	Forensic and Toxicology; drug; Micro...
OTC - Chloramphenicol	C ₁₂ H ₁₁ ClN ₂ O ₂	287.0671				56-76-1	56-76-1	2,2-Dichloro-1,1,1-trifluoroethane	6	Forensic and Toxicology; drug; Veterin...
OTC - Chloramphenicol	C ₁₂ H ₁₁ ClN ₂ O ₂	287.0671				56-76-1	56-76-1	2,2-Dichloro-1,1,1-trifluoroethane	6	Forensic and Toxicology; drug; Veterin...
Doxorubicin	C ₂₇ H ₃₉ N ₇ O ₁₁	543.2968				2321-92-8	2321-92-8	15-O-β-D-Glucopyranosyl-3,12-dihydroxy-10-methoxy-7,8-dihydro-6H-benzo[1,2-b:4,5-b']dioxepino[3,4-d]pyridine-6,11-dione	6	Forensic and Toxicology; drug; Micro...
Furazolidinone	C ₄ H ₅ N ₃ O	125.0431				138-26-3	138-26-3	1,2,4-Oxadiazole-5-carboxamide, 1,1-dioxide	6	Forensic and Toxicology; drug; Veterin...
Imazapyr	C ₁₀ H ₁₁ N ₃ O	197.0819				10026-61-9	10026-61-9	1,4-Dihydro-2,6-dimethyl-1H-imidazo[4,5-b]pyridine	6	Forensic and Toxicology; drug; Veterin...
Cyfluthrin A (Ectoparasiticide)	C ₂₂ H ₂₇ F ₃ O ₂	381.1617				10885-13-1	10885-13-1	1,1,1-Trifluoro-2,2,2-trifluoroethyl 2-cyano-3-phenoxyacetate	6	Forensic and Toxicology; drug; Veterin...
Ureic acid	C ₂ H ₄ N ₂ O	76.0471				124-08-2	124-08-2	2,6-Diisocyanato-1,3,5-triazine	5	Forensic and Toxicology; drug; Micro...
TC - Imazapyr	C ₁₀ H ₁₁ N ₃ O	197.0819				10026-61-9	10026-61-9	1,4-Dihydro-2,6-dimethyl-1H-imidazo[4,5-b]pyridine	5	Forensic and Toxicology; drug; Veterin...
Cyfluthrin	C ₂₂ H ₂₇ F ₃ O ₂	381.1617				10885-13-1	10885-13-1	1,1,1-Trifluoro-2,2,2-trifluoroethyl 2-cyano-3-phenoxyacetate	4	Forensic and Toxicology; drug; Veterin...
Zedonone	C ₁₈ H ₂₁ O ₃	283.1472				1726-32-4	1726-32-4	1,1,1-Trifluoro-2,2,2-trifluoroethyl 2-cyano-3-phenoxyacetate	4	Forensic and Toxicology; drug; Veterin...

Agilent's Mycotoxins PCDL ensures fast, customized method development.

MASSHUNTER EASES YOUR ICP-MS WORKFLOW

ICP-MS MassHunter Workstation for comprehensive control and analysis

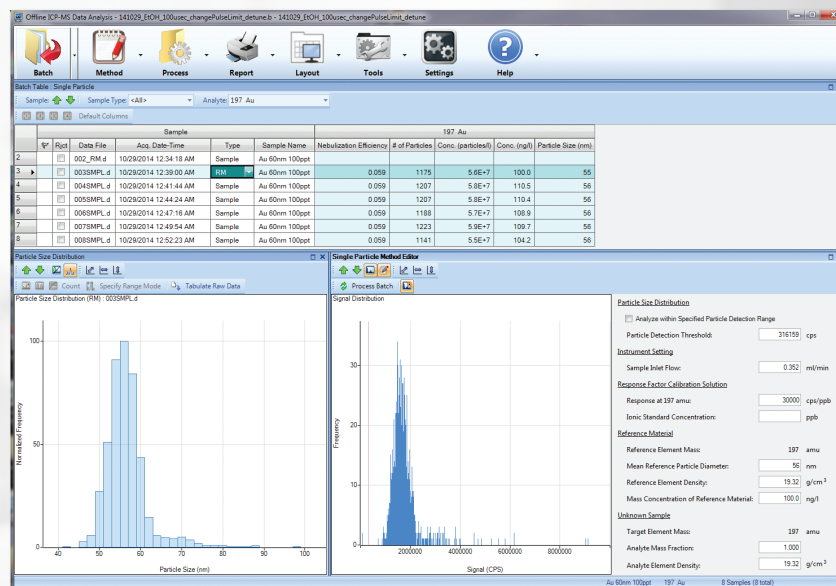
MassHunter software for ICP-MS includes complete instrument control, acquisition, and data analysis modules for stand-alone ICP-MS, as well as for hyphenated systems including HPLC and GC sample introduction. LabQC provides automatic flagging of outliers in quantitative analysis. Isotope ratio determination and time-resolved analysis are standard features, with optional modules that provide advanced functions such as real-time Intelligent QC, advanced chromatographic data analysis, and integration with Agilent OpenLAB Enterprise Content Manager.



Powerful qualitative and semi-quantitative ICP-MS data analysis. ICP-MS MassHunter Workstation provides comprehensive spectral processing tools for evaluating, comparing, and reporting information on uncalibrated analytes.

MassHunter single nanoparticle application mode

The fully integrated Agilent nanoparticle application module incorporates the entire process of nanoparticle determination into ICP-MS MassHunter software. The method wizard guides you through the automated creation of new nanoparticle methods for Agilent 7900 ICP-MS and 8800 Triple Quadrupole ICP-MS, and supports data acquisition in both FFF-ICP-MS and single nanoparticle modes. With a few mouse clicks, a complete analytical method, including optimized acquisition parameters, reference material values, and data analysis parameters, is set up and ready to run. The familiar "Batch at a Glance" table summarizes reference material and sample results for an entire batch. Paper or electronic reports including all data and graphics are automatically generated.



Nanoparticle application module final batch results are reported in tabular and graphical formats. Tab through individual samples in the table and review individual graphical results with powerful optimization tools.

OpenLAB—Agilent software gets you to the answers faster

MassHunter is part of Agilent's comprehensive, integrated OpenLAB software portfolio. From instrument control to enterprise content management, we recognize the critical role software plays in your lab's operation. We're working towards a single goal: to help you reduce the time, effort, and cost to get from raw data to final insight.

Other MassHunter literature:

Qualitative add-on modules:
 MassHunter Profiler Professional (MPP): 5990-4164EN
 Pathway Architect: 5991-1459EN
 Mass Profiler: 5991-5511EN
 Spectrum Mill: 5991-5250EN
 MassHunter and Skyline Integration: 5991-5248EN
 MassHunter Walkup: 5991-3836EN
 MassHunter BioConfirm: 5991-3643EN

Databases and PCDLs

METLIN: 5990-7854EN
 Mycotoxins PCDL overview: 5991-5691EN
 GC Q-TOF Pesticides PCDL Application Kit: 5991-5021EN
 All Ions MS/MS: Targeting screening and quantitation using Agilent TOF and Q-TOF LC/MS (technical overview): 5991-2465EN

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