Agilent Accurate-Mass 6500 Series Q-TOF
and 6200 Series TOF LC/MS Systems

The clearly better choice in TOF and Q-TOF LC/MS

Our measure is your success.

products | applications | software | services

Agilent Technologies

The unmatched confidence of Ultra High Definition Q-TOF Technology—plus the speed of Agilent's 1290 Infinity LC

Welcome to the power—and the certainty—of Ultra High Definition Q-TOF technology. They come together in the Agilent Accurate-Mass 6500 Series Q-TOF LC/MS and Agilent Accurate-Mass 6200 Series TOF LC/MS systems. And now the family is enhanced by the front-end speed, sensitivity, and chromatographic resolution of our new 1290 Infinity LC. So you can separate and identify more low abundance compounds faster, easier, and with higher confidence. Whether you are analyzing PTMs, profiling biomarkers, identifying metabolites, screening for pesticides, or characterizing intact proteins, Agilent TOF and Q-TOF solutions deliver the data quality demanded of the most critical science. You get:

The analytical performance you need to identify components in complex, real-world samples

The speed you need to realize the benefits of today's fastest UHPLC separations

The confidence you need to make better decisions, sooner

The data-mining tools you need to boost your lab's productivity and take full advantage of superior accurate-mass MS and MS/MS measurements

The advanced screening, profiling, and identification capabilities of Agilent's MassHunter software

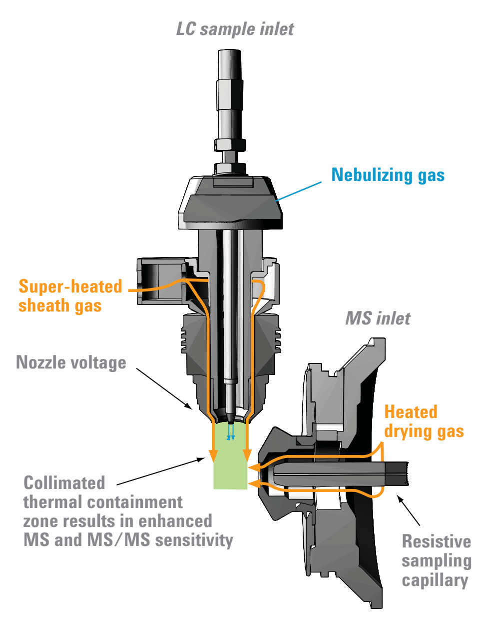
Agilent Accurate-Mass Time-of-Flight (TOF) and Quadrupole Time-of-Flight (Q-TOF) LC/MS systems *combine Ultra High Definition Q-TOF technology with advanced MassHunter Workstation software—plus the superior HPLC and UHPLC performance and flexibility of the new 1290 Infinity LC.*

Clearly better performance—by any measure

Through the use of Ultra High Definition Q-TOF technology, the 6200 and 6500 systems achieve industry-leading mass accuracy, dynamic range, and sensitivity without compromising data acquisition speed, mass range, or mass resolution—trade-offs that occur in competitive Q-TOF-based systems and even in more expensive Orbitrap mass analyzers.

It's a compelling proposition: you get the speed you need to keep up with today's ultra-fast UHPLC separations, plus the MS and MS/MS performance you need to get as much information as possible from the most challenging samples.

- **Sub ppm mass accuracy** improves confidence and reduces false positives.
- **Resolving power up to 40,000** separates compounds of interest from interferences.
- **Data acquisition rates up to 20 spectra per second** assures maximum data quality and compatibility with the fastest chromatography and high-throughput workflows.
- **Up to five orders of in-spectrum dynamic range** reveals trace-level targets even in the presence of vastly more abundant compounds.
- **High, femtogram-level sensitivity** finds impurities, metabolites, or biomarkers at extremely low concentrations.
- **Fast, scan-to-scan polarity switching** lets you analyze both positive and negative ions in a single experiment.
- **Automatic tuning and reliable delivery of an internal reference mass** ensures consistent mass accuracy and reliable elemental composition determination over a wide range of concentrations and *m/z*.



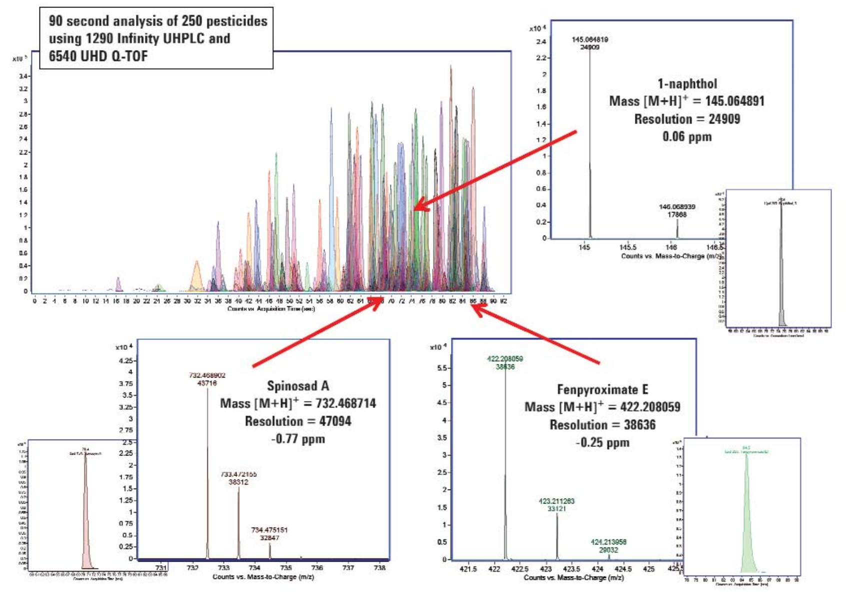
Agilent Jet Stream Technology increases LC/MS and LC/MS/MS sensitivity five-fold

Agilent Jet Stream Thermal Focusing technology significantly increases MS and MS/MS sensitivity by improving the spatial focusing of electrospray droplets. The innovative technology uses super-heated nitrogen to improve ion generation and desolvation for greater signal and reduced noise. This boosts sensitivity 5x or more for multiple applications, including the analysis of drug candidates and trace levels of food contaminants, metabolites, or biomarkers.

Exceptional MS and MS/MS performance—fully compatible with UHPLC

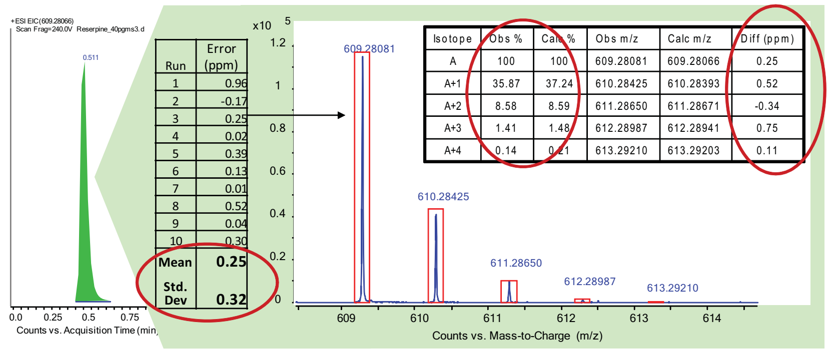
Whether you analyze small molecules or high MW proteins, the accurate-mass measurements of Agilent 6500 Series and 6200 Series systems give you greater certainty for screening, identification, and quantitation studies. Hardware innovations such as Agilent Jet Stream technology, ultra-fast analog-to-digital (ADC) acquisition, and automated reference mass delivery (now expanded for all Agilent liquid phase ion sources) all contribute to breakthrough performance improvements over previous generation TOF and Q-TOF instruments.

The result: exceptional analytical performance across multiple dimensions. Sensitivity, accurate mass, dynamic range, and resolution—all fully compatible with ultra-fast UHPLC separations.



Exceptional mass resolution helps you find more compounds

This example uses the 1290 Infinity LC with a ZORBAX Rapid Resolution High Definition (RRHD) column and 6540 Accurate-Mass Q-TOF. A 90-second assay of a suite of 250 pesticides yields excellent chromatographic and mass spectral resolution across the pesticide mass range. Three pesticide examples are detailed, representing low, mid, and high m/z.

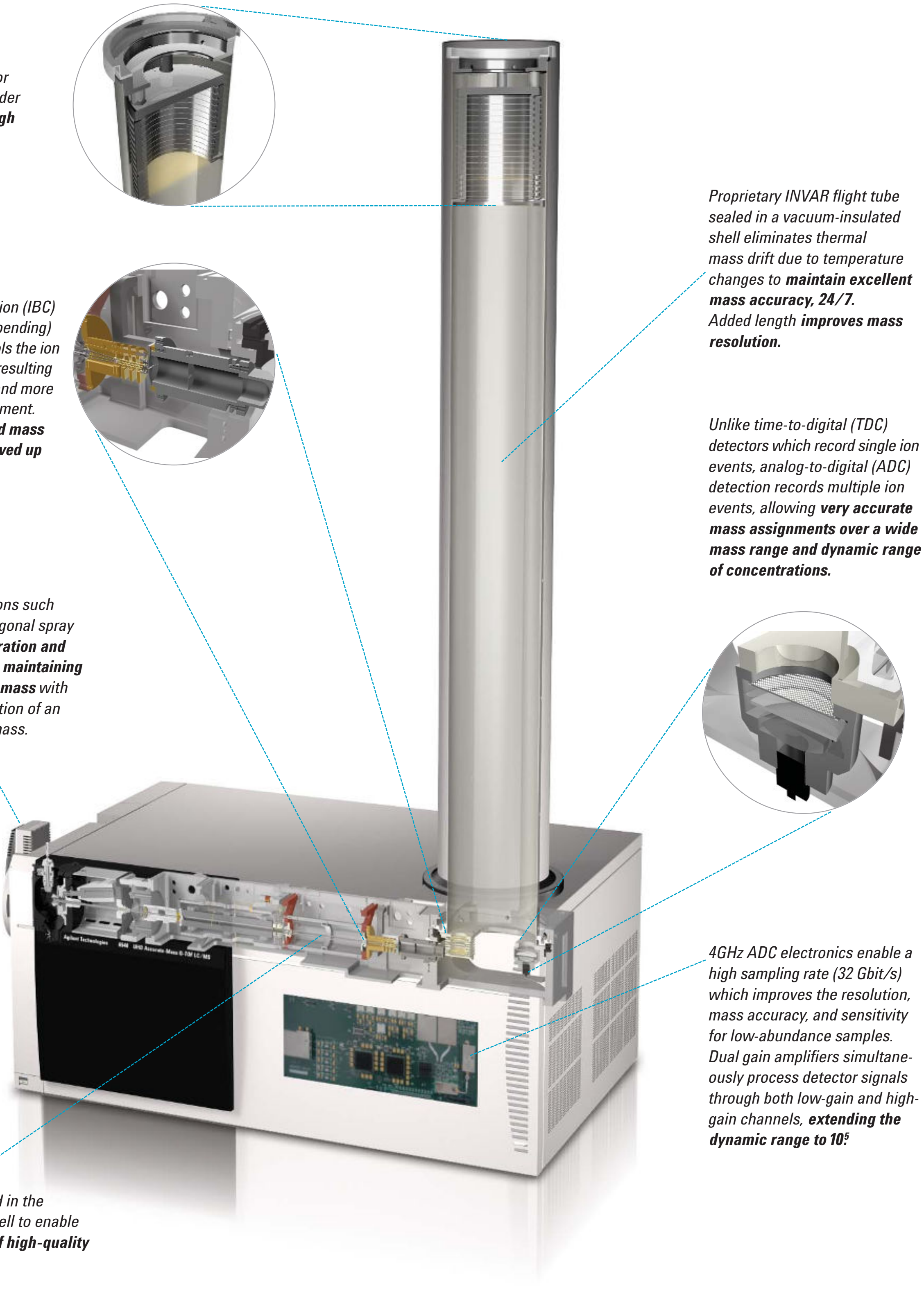


Run	Error (ppm)
1	0.96
2	-0.17
3	0.25
4	0.02
5	0.39
6	0.13
7	0.01
8	0.52
9	0.04
10	0.30
Mean	**0.25**
Std. Dev	**0.32**

Isotope	Obs %	Calc %	Obs m/z	Calc m/z	Diff (ppm)
A	100	100	609.28081	609.28066	0.25
A+1	35.87	37.24	610.28425	610.28393	0.52
A+2	8.58	8.59	611.28650	611.28671	-0.34
A+3	1.41	1.48	612.28987	612.28941	0.75
A+4	0.14	0.21	613.29210	613.29203	0.11

Exceptional mass accuracy improves analytical confidence

The innovative design of the 6500 Q-TOF collision cell and ion optics allows the same reference mass calibration to be used for both MS and MS/MS. The resulting MS mass accuracy—in this example, 0.32 ppm—and precise isotopic ratios greatly improve confidence in molecular formula generation. Excellent isotopic ratio fidelity is shown for 10 replicate reserpine injections at 40 pg on-column.



Dual-stage ion mirror improves second-order time focusing for ***high mass resolution.***

Ion Beam Compression (IBC) Technology (patent pending) compresses and cools the ion beam up to 10-fold, resulting in fewer ion losses and more precise mass assignment. ***Mass resolution and mass accuracy are improved up to 200 percent.***

Ion source innovations such as proprietary orthogonal spray ***maximize ion generation and reduce noise, while maintaining excellent accurate mass*** *with automated introduction of an internal reference mass.*

Ions are accelerated in the hexapole collision cell to enable ***faster generation of high-quality MS/MS spectra.***

Proprietary INVAR flight tube sealed in a vacuum-insulated shell eliminates thermal mass drift due to temperature changes to ***maintain excellent mass accuracy, 24/7.***
Added length ***improves mass resolution.***

Unlike time-to-digital (TDC) detectors which record single ion events, analog-to-digital (ADC) detection records multiple ion events, allowing ***very accurate mass assignments over a wide mass range and dynamic range of concentrations.***

4GHz ADC electronics enable a high sampling rate (32 Gbit/s) which improves the resolution, mass accuracy, and sensitivity for low-abundance samples. Dual gain amplifiers simultaneously process detector signals through both low-gain and high-gain channels, ***extending the dynamic range to*** 10^5

Clearly better productivity—for any application

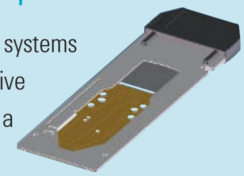
Sometimes productivity is all about speed. Sometimes it's all about data quality. And often, it's about both. Agilent TOF and Q-TOF solutions offer a combination of unbeatable separation speed and resolution, superior qualitative MS and MS/MS capabilities, and powerful MassHunter data mining software—so they can match any productivity challenge your lab may have.

Agilent 1290 Infinity LC System: An infinitely better liquid chromatography platform

The 1290 Infinity LC complements the performance of Ultra High Definition Q-TOF technology and allows you to optimize your separations for maximum productivity. ZORBAX Rapid Resolution High Definition (RRHD) columns provide the separating power for excellent UHPLC results. Take full advantage of fast chromatography for high-throughput analysis. For very complex samples, use the 1290 Infinity LC system's unmatched peak capacity and chromatographic resolution to minimize co-elution and ion suppression effects.

***The Agilent 1290 Infinity LC** delivers unprecedented, best-in-class speed, resolution, and sensitivity—for better overall HPLC and UHPLC performance.*

HPLC-Chip/MS technology offers highest sensitivity for small-volume samples



The Agilent 6500 Series and 6200 Series systems are also fully compatible with our innovative 1200 Series HPLC-Chip/MS technology—a plug-and-play alternative to complicated nanoflow LC separations. The easy-to-use technology combines the sample enrichment and separation columns of a 1200 Series Nanoflow LC system with an integrated nanospray tip—all on a single, reusable microfluidic chip about the size of a microscope slide. It delivers robust, ultra-sensitive results and is especially well-suited for protein and peptide applications using small sample volumes.

- Highest sensitivity ensures low-level sample fidelity.
- Narrower, better-defined chromatographic peaks reduce MS complexity for more confident compound identification.
- The new HPLC-Chip II features a new carbon-ion-implanted filter resulting in optimal chip-to-chip and run-to-run reproducibility for maximum productivity.
- More reliable nanospray MS facilitates biomarker discovery and validation, intact monoclonal antibody characterization, phosphopeptide analysis, and small molecule analysis, such as DMPK.

MassHunter software amplifies your productivity

From instrument setup to final report, Agilent's MassHunter Workstation software is designed to make all of your MS analyses faster, easier, and more productive. Data analysis tools let you quickly find, compare, and identify compounds in complex matrices. Compound-centric data-mining and navigation capabilities streamline and simplify MS data analyses.

One easy-to-learn interface handles all of your basic qualitative and quantitative analysis tasks and also integrates seamlessly with Agilent's powerful application-specific workflow software.

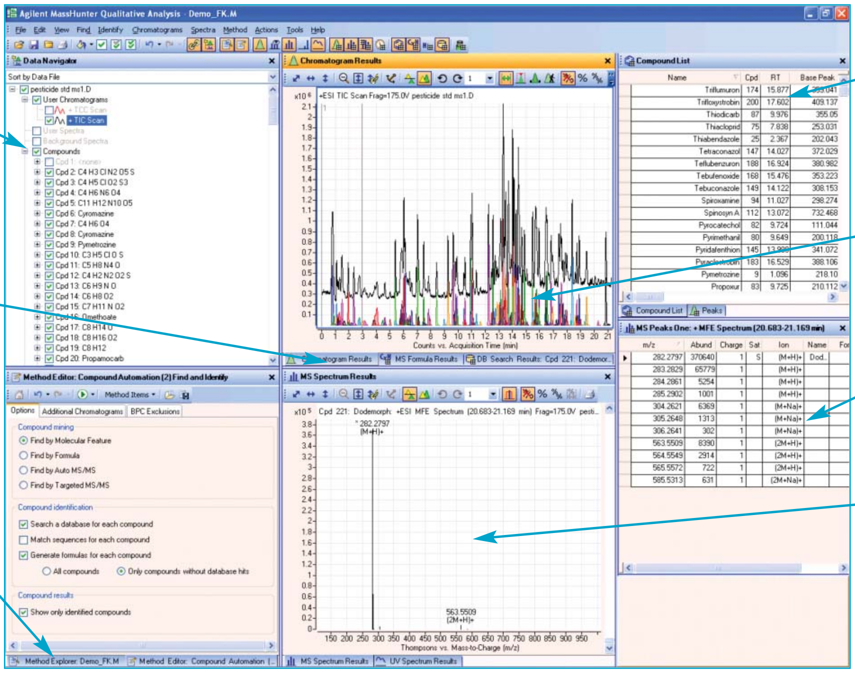
If it's there, MassHunter will help you find, compare, and identify it. Proprietary algorithms enable comprehensive data mining to bring the highest level of certainty to the confirmation and identification of unknowns.

Integrated, application-driven database and library searching. To enhance your productivity—and to make compound identification easier—MassHunter software lets you perform automated, accurate-mass searches against METLIN and other public and private databases. Pesticide, forensic, toxicology, and other small molecule compounds can be searched using accurate mass and retention time or by generating molecular formulas from accurate-mass MS or MS/MS data.

Compound-centric data navigation and selection

Detailed Molecular Formula Generation and accurate mass databases search results

Method Editor and Explorer



Sort by Data File

- pesticide std ms1.D
  - User Chromatograms
    - + TCC Scan
    - + TIC Scan
  - User Spectra
  - Background Spectra
  - Compounds
    - Cpd 1: <none>
    - Cpd 2: C4 H3 Cl N2 O5 S
    - Cpd 3: C4 H5 Cl O2 S3
    - Cpd 4: C4 H6 N6 O4
    - Cpd 5: C11 H12 N10 O5
    - Cpd 6: Cyromazine
    - Cpd 7: C4 H6 O4
    - Cpd 8: Cyromazine
    - Cpd 9: Pymetrozine
    - Cpd 10: C3 H5 Cl O S
    - Cpd 11: C5 H8 N4 O
    - Cpd 12: C4 H2 N2 O2 S
    - Cpd 13: C6 H9 N O
    - Cpd 14: C6 H8 O2
    - Cpd 15: C7 H11 N O2
    - Cpd 16: Omethoate
    - Cpd 17: C8 H14 O
    - Cpd 18: C8 H16 O2
    - Cpd 19: C8 H12
    - Cpd 20: Propamocarb

Method Editor: Compound Automation (2) Find and Identify

Options | Additional Chromatograms | BPC Exclusions

Compound mining
● Find by Molecular Feature
○ Find by Formula
○ Find by Auto MS/MS
○ Find by Targeted MS/MS

Compound identification
☑ Search a database for each compound
☐ Match sequences for each compound
☑ Generate formulas for each compound
○ All compounds ● Only compounds without database hits

Compound results
☑ Show only identified compounds

Compound List

Name	Cpd	RT	Base Peak
Triflumuron	174	15.877	[illegible]
Trifloxystrobin	200	17.602	409.137
Thiodicarb	87	9.976	355.05
Thiacloprid	75	7.838	253.031
Thiabendazole	25	2.367	202.043
Tetraconazol	147	14.027	372.029
Teflubenzuron	188	16.924	380.982
Tebufenoxide	168	15.476	353.223
Tebuconazole	149	14.122	308.153
Spiroxamine	94	11.027	298.274
Spinosyn A	112	13.072	732.468
Pyrocatechol	82	9.724	111.044
Pyrimethanil	80	9.649	200.118
Pyridafenthion	145	[illegible]	341.072
Pyraclostrobin	183	16.529	388.106
Pymetrozine	9	1.096	218.10
Propoxur	83	9.725	210.112

MS Peaks One: + MFE Spectrum (20.683-21.169 min)

m/z	Abund	Charge	Sat	Ion	Name	For
282.2797	370640	1	S	(M+H)+	Dod..	
283.2829	65779	1		(M+H)+		
284.2861	5254	1		(M+H)+		
285.2902	1001	1		(M+H)+		
304.2621	6369	1		(M+Na)+		
305.2648	1313	1		(M+Na)+		
306.2641	302	1		(M+Na)+		
563.5509	8390	1		(2M+H)+		
564.5549	2914	1		(2M+H)+		
565.5572	722	1		(2M+H)+		
585.5313	631	1		(2M+Na)+		

List of compounds with best molecular formulas and accurate mass databases search hits

Overlaid compound chromatograms for each individual compound

Mass peak list with identified ion species for each compound

Compound mass spectrum with a theoretical isotope pattern overlaid for generated formulas

Easily find, compare, and identify compounds in qualitative analysis. *MassHunter Workstation makes it easy to create, organize, navigate, store, and report results on a compound-by-compound basis.*

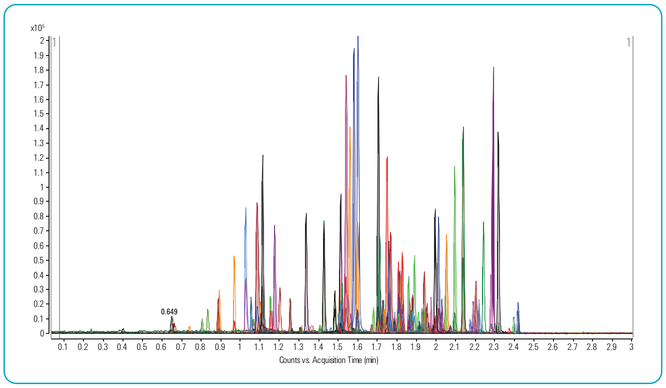
Automatically find, compare, identify, and quantitate compounds *using MassHunter Workstation's unique compound-centric data processing.*

To learn more about Agilent 6500 Q-TOF and 6200 Series TOF LC/MS solutions, visit www.agilent.com/chem/qtof

Powerful, easy-to-use solutions for food safety and environmental analysis

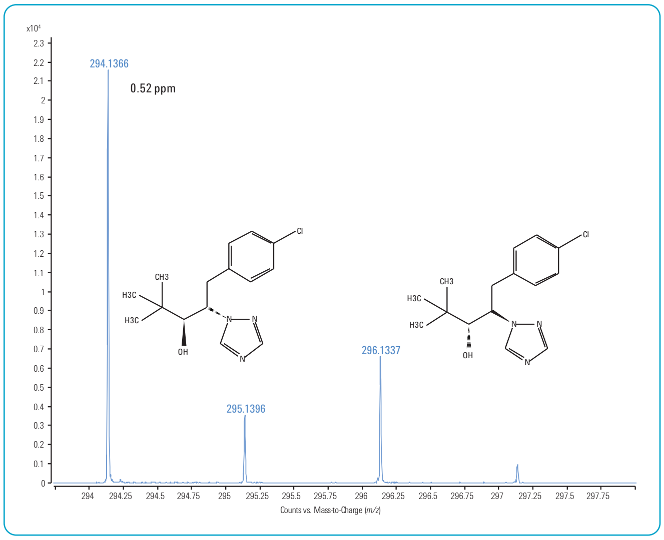
Agilent's combination of ultra-fast spectral acquisition, wide dynamic range, and superior mass accuracy and mass resolution lets you screen for hundreds of compounds in a single analysis—even in the most complex matrices. MassHunter software locates sample components and automatically searches your public and private databases, rapidly providing high-confidence answers. New Agilent application kits—including methods, chemicals, compound databases, and more—help you spend less time on setup and configuration and more time generating expert results.

Ultra-fast screening and identification of pesticides



Q-TOF identification of 100 pesticides in less than three minutes. *Superior peak capacity and fast MS acquisition lets you resolve large numbers of pesticides and ensures high confidence in compound identification. The fast acquisition capability of the Q-TOF allows considerably shorter run times while still acquiring full spectral data. (1290 Infinity LC using a ZORBAX RRHD column and 6540 Accurate-Mass Q-TOF)*

High resolution MS, sub 1 ppm mass accuracy, and isotope peak fidelity at 10 scans per second



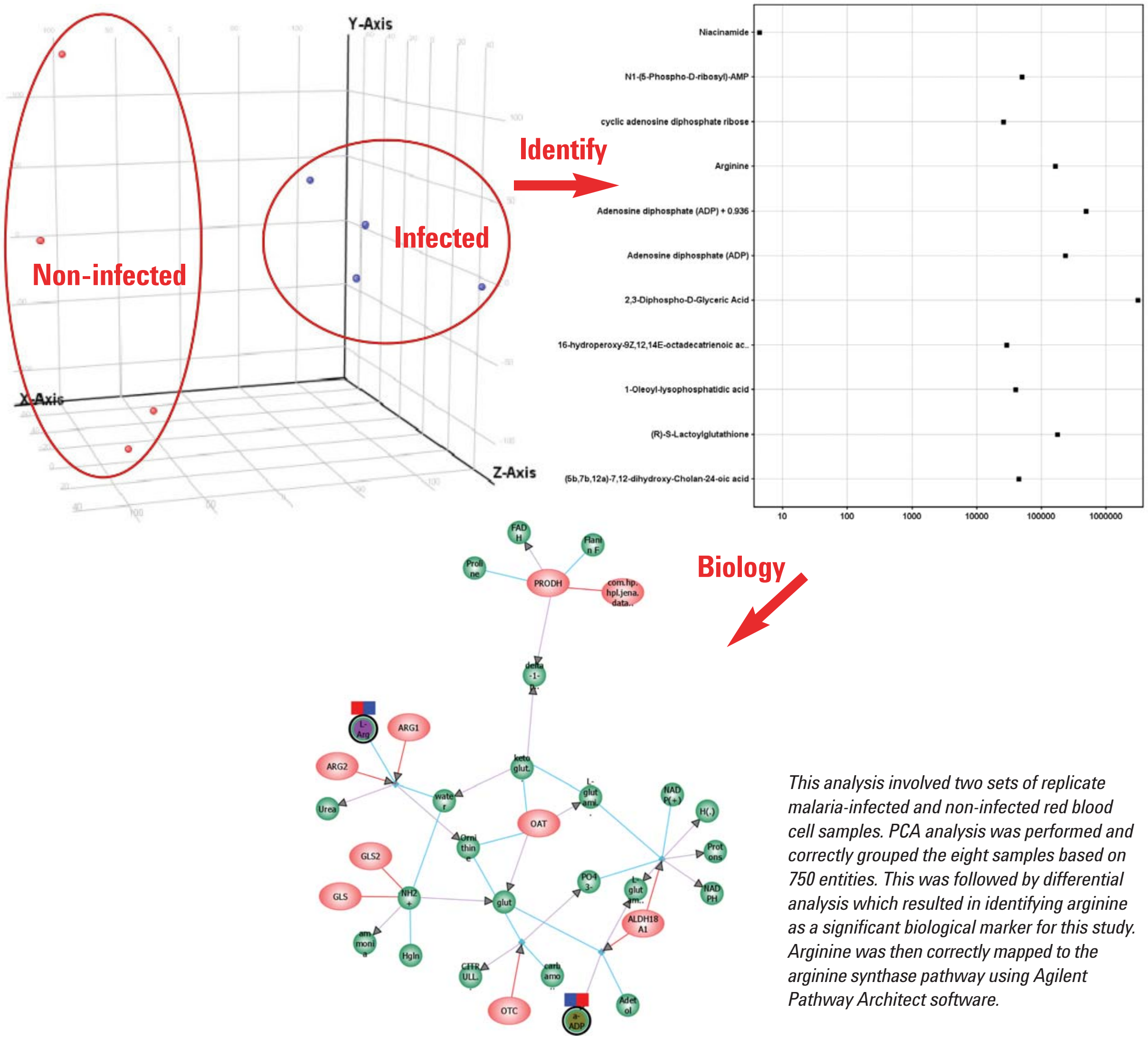
Screening for thousands of pesticides in three minutes. *In this example, 10 data points are collected across each one-second wide LC peak, allowing thousands of pesticides to be screened in the three-minute timeframe.*

Powerful workflows find more biomarkers, more quickly

Agilent's Ultra High Definition Q-TOF technology gives you the power to quickly find differences in expression levels between sample groups and identify potential biomarkers in your accurate-mass LC/MS data. Together with integrated software solutions—such as Agilent's METLIN Personal Metabolite Database and Mass Profiler Professional—the platform provides tools to help understand complex biological systems.

Superior TOF sensitivity and five orders of dynamic range help you detect very low-abundance metabolites in the presence of vastly more abundant compounds. Sub-ppm MS typical mass accuracy generates higher confidence in compound identification and reduces false positives when searching with Agilent's METLIN Personal Metabolite Database of over 23,000 endogenous and exogenous metabolites, lipids, and di- and tripeptides.

A comprehensive suite of metabolomics data mining tools for profiling, multivariate analysis, identification, and pathway elucidation



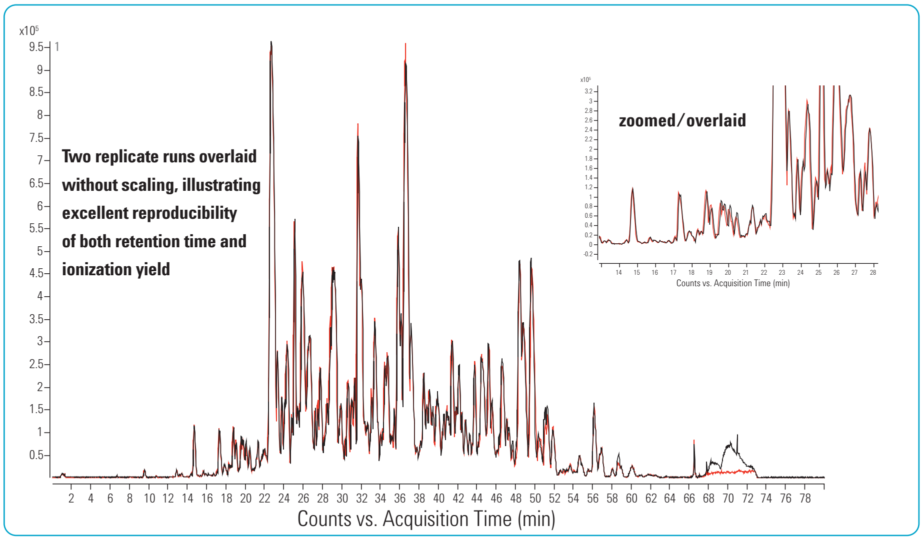
This analysis involved two sets of replicate malaria-infected and non-infected red blood cell samples. PCA analysis was performed and correctly grouped the eight samples based on 750 entities. This was followed by differential analysis which resulted in identifying arginine as a significant biological marker for this study. Arginine was then correctly mapped to the arginine synthase pathway using Agilent Pathway Architect software.

To learn more about Agilent 6500 Q-TOF and 6200 Series TOF LC/MS solutions, visit **www.agilent.com/chem/qtof**

High-confidence biomolecule identification, characterization, and quantitation

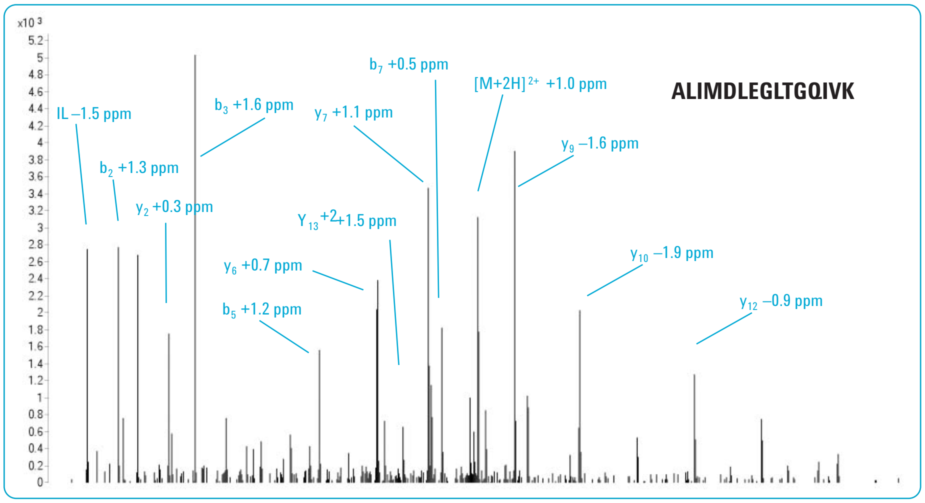
Agilent's 1200 Series HPLC-Chip/MS system provides fast, highly reproducible nanoflow LC separations—critical for achieving good results in differential analysis, and an ideal complement to the high spectral quality of the Accurate-Mass Q-TOF platform. Wide dynamic range, coupled with excellent mass accuracy and mass resolution, optimizes profiling performance allowing you to uncover more low-abundance compounds and to see peptides and proteins at both high and low levels of concentration.

Excellent MS reproducibility


Two replicate runs overlaid without scaling, illustrating excellent reproducibility of both retention time and ionization yield

Overlaid chromatograms are shown for two replicate runs of a tryptic digest of an SEC fraction from a Schizosaccharomyces pombe sample. The results show the high level of reproducibility of both retention time and ionization yield. (Agilent HPLC-Chip/MS and 6540 Accurate-Mass Q-TOF)

Superior MS/MS mass accuracy


ALIMDLEGLTGQIVK

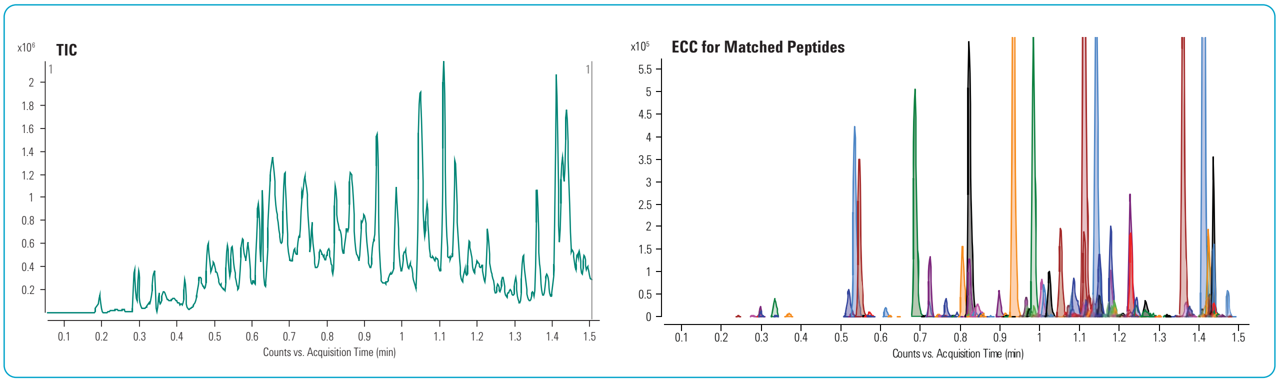
An MS/MS spectrum is shown for a peptide, ALIMDLEGLTGQIVK, from Schizosaccharomyces pombe. The average product ion mass accuracy was 2.3 ppm. All b- and y- ions from the peptide are shown with corresponding mass accuracy values. (Agilent HPLC-Chip/MS and 6538 Accurate-Mass Q-TOF)

Reliable confirmation of intact proteins

Full characterization of proteins of interest—including details about molecular composition and structural variations—requires in-depth, accurate analysis of both the intact and digested forms. The accurate-mass MS and MS/MS measurements of Agilent's Q-TOF platform ensure higher confidence in identifying intact proteins. The system's high resolution resolves charge states and gives you the power to pinpoint small changes in structure from post-translational modifications, chemical degradation, and modification.

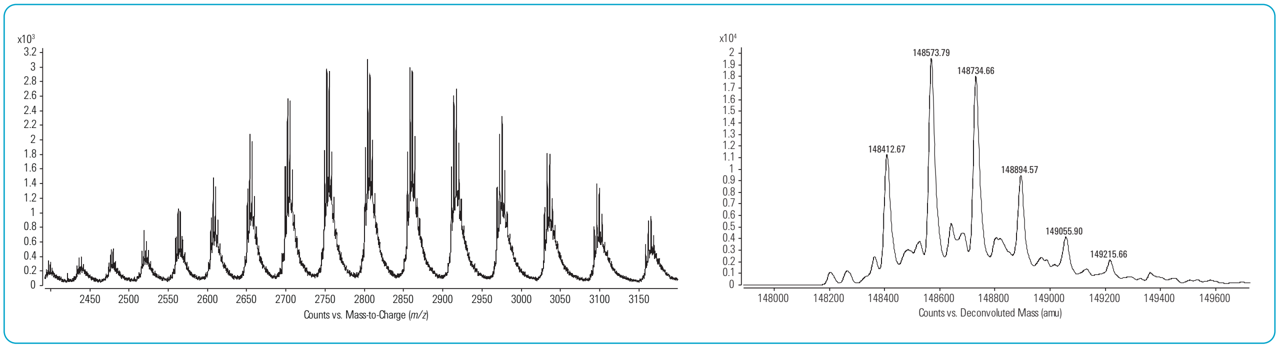
MassHunter BioConfirm software provides optimized mass spectral deconvolution and a sequence editor/matcher for peptide mapping, as well as the prediction and confirmation of protein modifications, resulting in accelerated characterization of recombinant proteins and synthetic peptides.

100 percent sequence coverage of monoclonal antibody digest



Complete mAb sequence coverage in less than two minutes. *This example shows extracted compound chromatograms (ECC) for peptides matched to the IgG sequence; for both light and heavy chains, 100 percent sequence coverage was obtained. At a flow rate of 1.6 mL/min with system pressure of >1100 bar, analysis time was under two minutes. (Agilent 1290 Infinity LC using a Poroshell 120 column and 6530 Accurate-Mass Q-TOF)*

MS measurement and deconvolution of intact antibody



MS spectrum of deglycosylated ANTI-FLAG antibody following a 600 pg (4 fmol) injection on column. The deconvoluted spectrum on the right shows six different major glycoforms. Analysis was performed using HPLC-Chip/MS with 43 mm ZORBAX SB 300-C18 chip. (Agilent HPLC-Chip/MS and 6530 Accurate-Mass Q-TOF)

Workflow-driven applications add power and productivity

To maximize your lab's productivity, easy-to-use, application-specific software solutions can be seamlessly integrated into MassHunter Workstation. These include:

Mass Profiler Professional
Powerful chemometrics software package that fully exploits the high information content of accurate-mass MS data

Spectrum Mill for MassHunter Workstation
Protein identification, relative quantitation, characterization

MassHunter BioConfirm Software
Intact protein characterization and oligonucleotide analysis

MassHunter Metabolite ID Software
Drug metabolite identification

Personal Compound Database & Library Software

- MassHunter Personal Forensic and Toxicology Database
  Over 7,000 compounds available
- MassHunter Personal Pesticide Database
  Over 1,600 compounds available
- Agilent METLIN Personal Metabolite Database
  Most comprehensive endogenous metabolite database available—includes over 23,000 compounds including 8,000 lipids

Agilent Services keep your lab running at peak productivity

With a 98% customer satisfaction rating, Agilent's service engineers are the most respected—and best-trained—in the industry. Whether you need support for a single instrument or a multi-lab, multi-vendor operation, we can help you solve problems quickly, increase your uptime, and optimize your lab's resources. Through a selection of service plans tailored to your lab's needs and budget, we provide:

- On-site preventive maintenance that ensures dependable system operation and minimizes unplanned downtime
- Remote diagnostic and monitoring capabilities that give you additional "uptime insurance"
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- Expert installation, familiarization, and advanced training to get you up and running as quickly as possible and to make sure you get the most from your new Agilent equipment

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Printed in USA February 10, 2010
5990-4052EN

Agilent Technologies