Agilent 6210 Time-of-Flight LC/MS

Turning samples into answers

Agilent Technologies

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Whether you analyze drug candidates or environmental samples, proteins or synthetic peptides, the Agilent 6210 Time-of-Flight LC/MS has the outstanding analytical performance; powerful, application-specific software; and ease of use you need to turn every sample into answers.

Industry-leading performance...

The Agilent 6210 Time-of-Flight LC/MS has the exceptional analytical performance you need. It:

- Provides greater analytical confidence thanks to 2-ppm mass accuracy
- Resolves complex mixtures, distinguishing compounds of interest from interferences
- Simultaneously identifies high- and low-abundance components using its wide dynamic range
- Identifies unresolved components, even in narrow chromatographic peaks, with its ultra-fast data acquisition
- Detects even low-level components through outstanding sensitivity
- Acquires more information from unknowns by switching polarity spectrum-to-spectrum; especially when paired with the multimode source

...achieved more easily

While mass accuracy and overall analytic performance of the 6210 TOF are superlative, operation is surprisingly simple. Automated tuning and fully automated delivery of an internal reference mass standard ensure maximum performance with minimum effort. Application-specific software optimizes results and maximizes productivity for both large-molecule and small-molecule applications. And software to facilitate walk-up operation and remote data review can further ease operation.

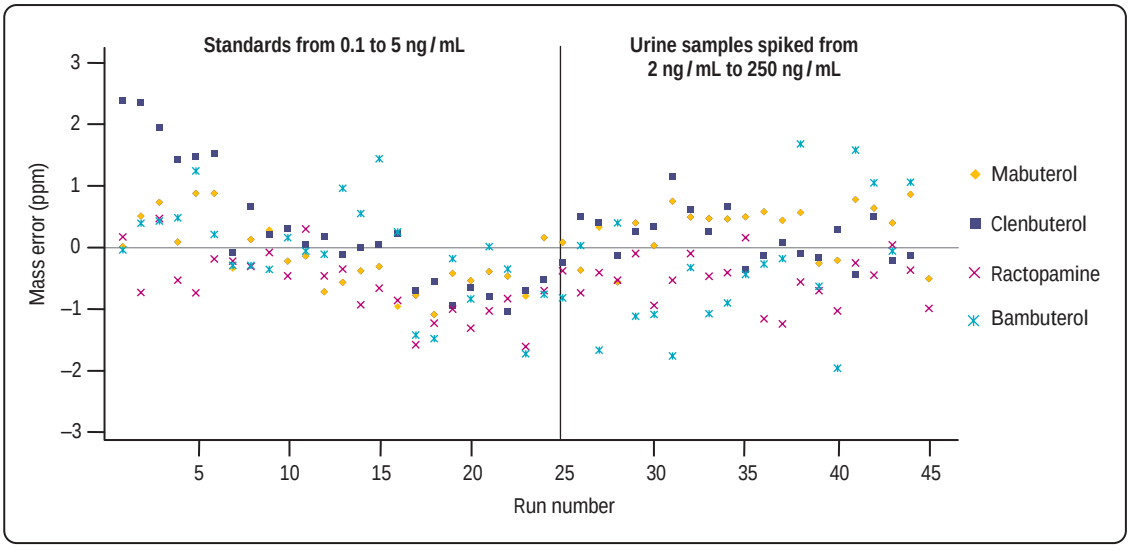
Superior mass accuracy and mass resolution increase confidence

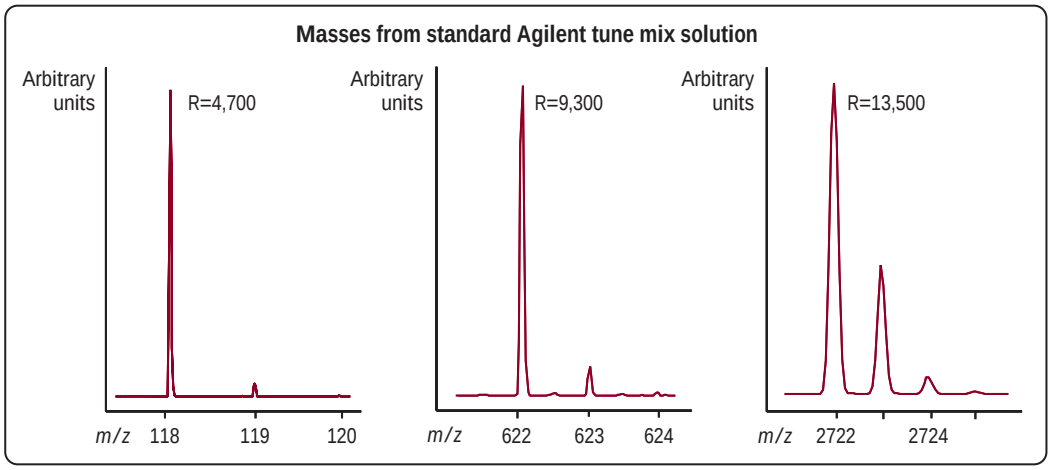
The 6210 TOF was designed from the ground up to simultaneously provide you with excellent mass accuracy, mass resolution, dynamic range, and spectral acquisition rate.

For lower-molecular-weight compounds, the 2-ppm mass accuracy of the 6210 can positively confirm elemental composition and identify unknowns. For higher-molecular-weight compounds, it can dramatically limit the number of likely candidates, so you can make a positive identification based on a combination of accurate mass measurements and complementary information.

The outstanding resolving power of the 6210 minimizes the chance that a mass peak of interest will be merged with an interfering ion from the sample or background. The 6210 TOF can distinguish many compounds with identical nominal masses and readily identifies protein variants attributable to post-translational modifications or point mutations.

The 6210 TOF routinely measures masses to accuracies of 1–2 ppm, as shown by results of this 18-hour sequence of β_2-agonist standards and spiked urine samples

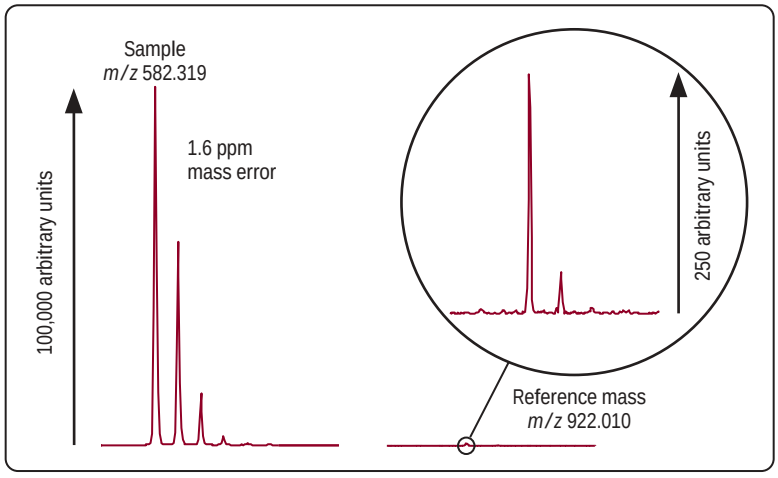




The 6210 TOF's high resolving power ensures the best chance of distinguishing all sample components

Wide dynamic range helps identify minor components and simplifies operation

Agilent's 6210 TOF supplies a stunning 3+ orders-of-magnitude in-spectrum dynamic range—without employing beam attenuation that robs some other TOF instruments of sensitivity. This dynamic range enables you to identify less abundant compounds in the presence of significantly more abundant compounds, even within a single spectrum. It also facilitates unattended "walk-up" access because there is no need to precisely match sample concentration to the detection range of the instrument.



Wide dynamic range ensures that both major and minor components are identified, and facilitates use of an internal standard

Fast spectral acquisition matches your fast chromatography

At 40 spectra per second, the 6210 provides more than enough data for reliable qualitative and quantitative results—even when you use the fastest chromatography. You can identify unresolved or poorly resolved components even in narrow one- to two-second-wide peaks. Fast spectral acquisition also ensures more accurate peak area measurements for more accurate quantitation.

Compatible with the widest range of applications

With the appropriate Agilent LC, ion source, and software, the Agilent 6210 Time-of-Flight LC/MS will provide answers to many analytical challenges: from identity confirmation for products of synthetic chemistry to fast expression profiling of complex protein samples.

A source for every analysis

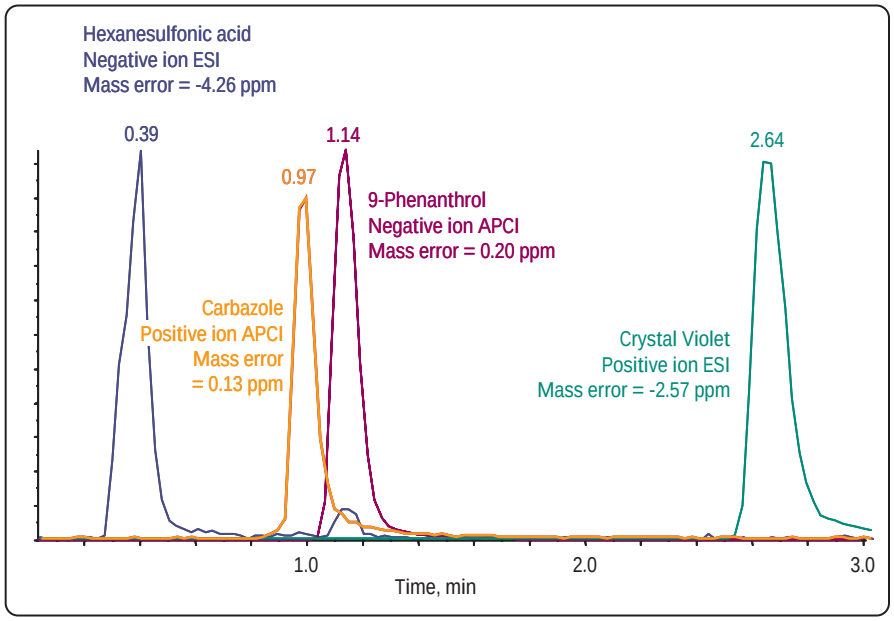
The 6210 TOF offers one of the widest selections of ion sources, including dual-nebulizer sources. Dual-nebulizer sources maximize both mass accuracy and ease of use by introducing an internal reference mass standard through a second nebulizer dedicated to that task. This also facilitates automated tuning—a rarity in TOF instruments.

- Dual-nebulizer electrospray (ESI) for all-around performance
- Dual-nebulizer nanospray provides extra sensitivity
- APCI for less polar samples that do not ionize well by electrospray
- APPI for compounds that do not respond well to ESI and APCI
- CE-TOF interface to take advantage of the resolving power of CE
- PDF-MALDI* for high-throughput proteomics
- Multimode increases productivity by acquiring ESI and APCI data simultaneously
- HPLC-Chips and HPLC-Chip Cube MS interface for the ultimate in separation and sensitivity

Dual-nebulizer ESI ion source ensures maximum mass accuracy with minimum effort

HPLC-Chip Cube MS interface maximizes sensitivity and convenience

Multimode ion source can double throughput and productivity



In a single run, a 6210 TOF with spectrum-to-spectrum polarity switching and a multimode ion source identifies four compounds that each respond to a different combination of ionization method and ionization polarity

*The PDF-MALDI source is a Class I Laser Product

Simplified analysis of small molecules

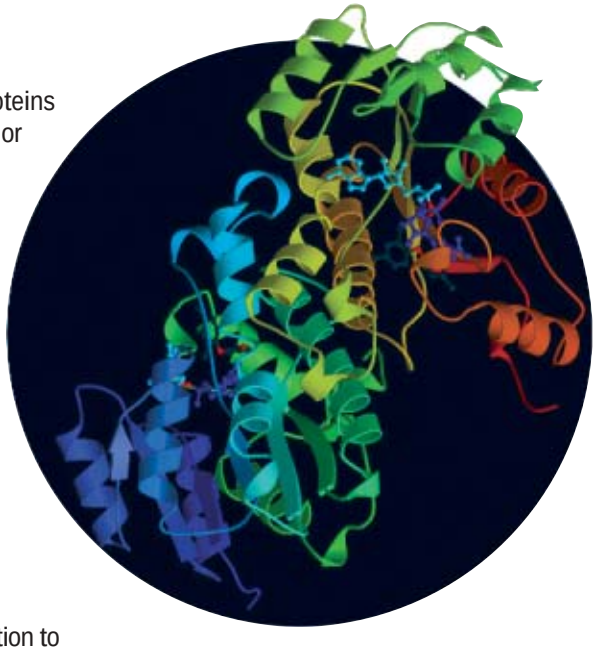
If you perform high-throughput screening, impurity analyses, or environmental or forensic analyses, the 6210 TOF offers:

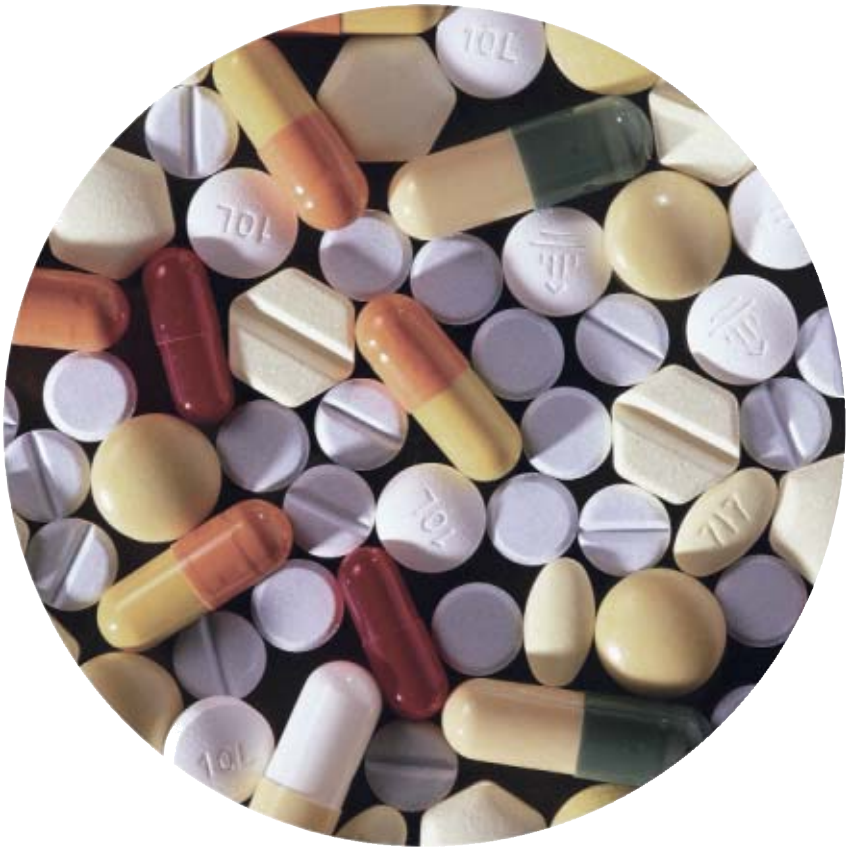
- Empirical formula confirmation software for fast, positive confirmation of expected compounds
- Empirical formula generation software that leverages the power of accurate mass measurements to identify impurities and other unknowns
- Feature extraction and correlation algorithm that improves the accuracy of empirical formula determination and database searching

Improved analysis of biomolecules

If your research involves proteins and peptides, either natural or synthetic, the 6210 can be paired with:

- MassHunter Bioconfirmation software to confidently confirm protein and peptide identities and identify both unexpected variants and true unknowns
- MassHunter Profiling software that applies optimized tools for compound location and data visualization to differential expression studies and biomarker discovery





Enhanced productivity and ease of use

Additional software is available to make the power of TOF accessible to more researchers and simplify data review for everyone.

- MassHunter Easy Access software enables simple, walk-up operation and is ideal for shared-instrument, multiuser environments
- Data Browser software facilitates data review on remote PCs without TOF software

These packages are compatible with both small-molecule and biomolecule applications and software.

Easily confirm small molecule identities and identify unknowns

The 2-ppm mass accuracy of the 6210 TOF is great for both confirmation of compound identities and the identification of unknowns. In many cases, the accurate mass measurement alone is sufficient. In other cases, it narrows the possible candidates enough that confirmation or identification becomes much easier.

Quickly confirm compound identities

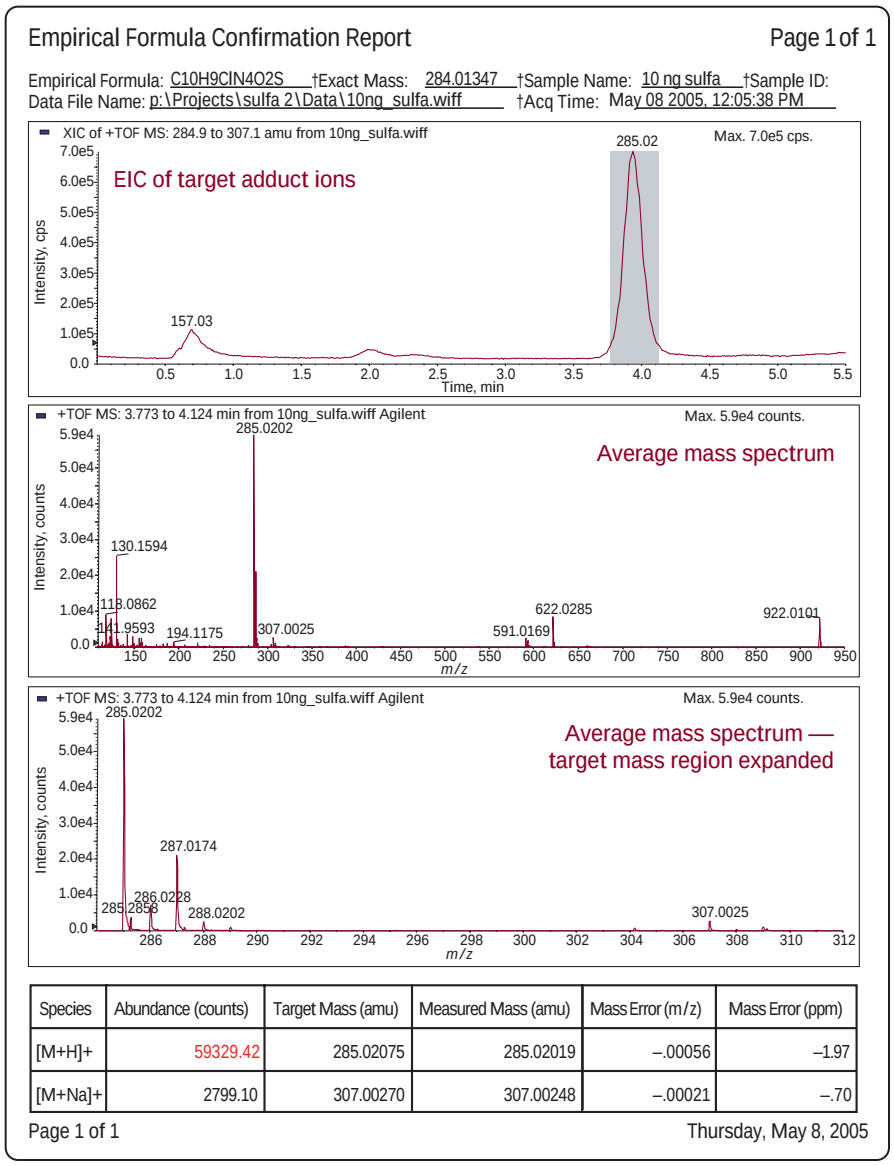
The empirical formula confirmation software allows you to quickly and easily verify the presence of expected compounds. Starting from an empirical formula, it reviews extracted spectra, looking for expected masses. It accounts for neutral losses, adducts, and other common modifications. The program generates a single-page confirmation report for each target compound.

Identify unknowns with empirical formula generation software

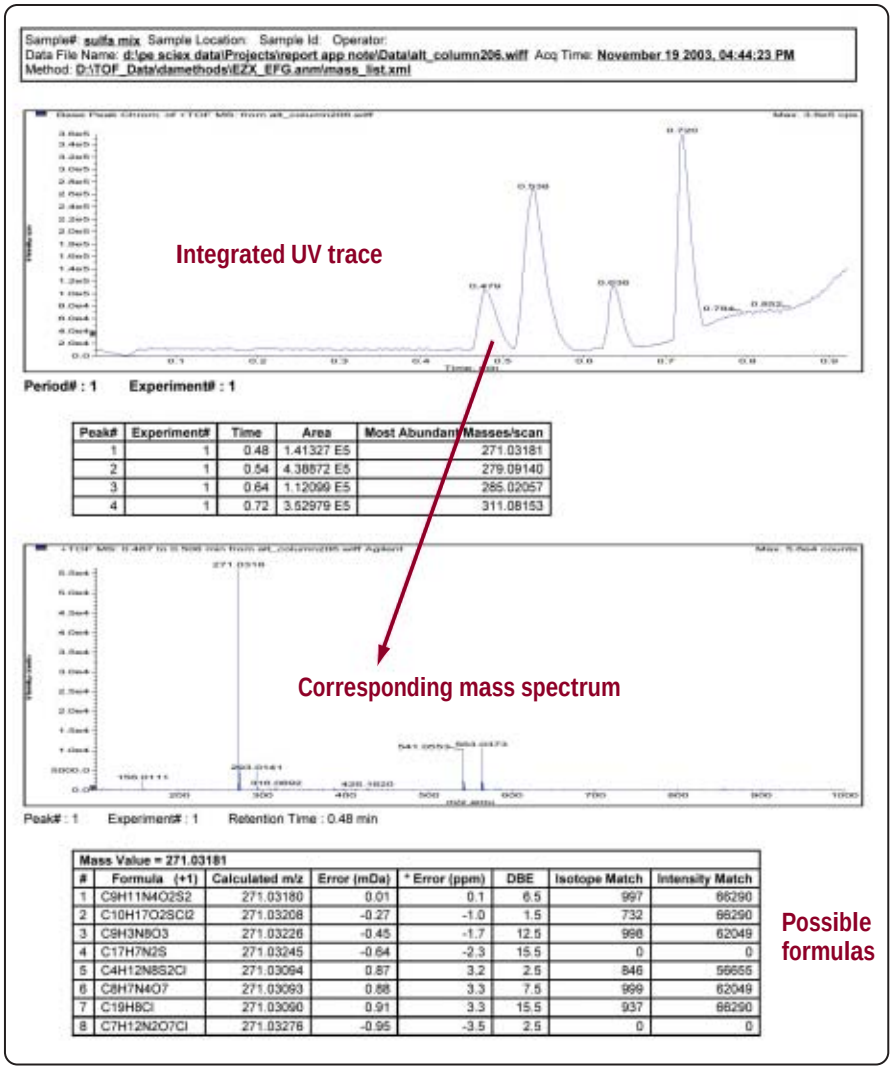
From the results in the mass list, you can generate a list of likely empirical formulas for each unknown. You can customize formula generation using a wide range of parameters including:

- Mass tolerance
- List of possible elements
- Minimum and maximum values for each element
- Electron state (odd or even)
- Charge state
- Maximum error range
- Maximum number of hits

Results can be sorted by isotope ratio fit or mass error.



The empirical formula confirmation report displays essential result information for each target compound



Sample# sulfa mix Sample Location: Sample Id: Operator:
Data File Name: d:\pe sciex data\Projects\report app note\Data\alt_column206.wiff Acq Time: November 19 2003, 04:44:23 PM
Method: D:\TOF_Data\damethods\EZX_EFG.anm\mass_list.xml

Period# : 1 Experiment# : 1

Peak#	Experiment#	Time	Area	Most Abundant Masses/scan
1	1	0.48	1.41327 E5	271.03181
2	1	0.54	4.38872 E5	279.09140
3	1	0.64	1.12099 E5	285.02057
4	1	0.72	3.52979 E5	311.08153

Peak# : 1 Experiment# : 1 Retention Time : 0.48 min

Mass Value = 271.03181

#	Formula (+1)	Calculated m/z	Error (mDa)	* Error (ppm)	DBE	Isotope Match	Intensity Match
1	C9H11N4O2S2	271.03180	0.01	0.1	6.5	997	66290
2	C10H17O2SCl2	271.03208	-0.27	-1.0	1.5	732	66290
3	C9H3N8O3	271.03226	-0.45	-1.7	12.5	998	62049
4	C17H7N2S	271.03245	-0.64	-2.3	15.5	0	0
5	C4H12N8S2Cl	271.03094	0.87	3.2	2.5	846	59655
6	C8H7N4O7	271.03093	0.88	3.3	7.5	999	62049
7	C19H8Cl	271.03090	0.91	3.3	15.5	937	66290
8	C7H12N2O7Cl	271.03276	-0.95	-3.5	2.5	0	0

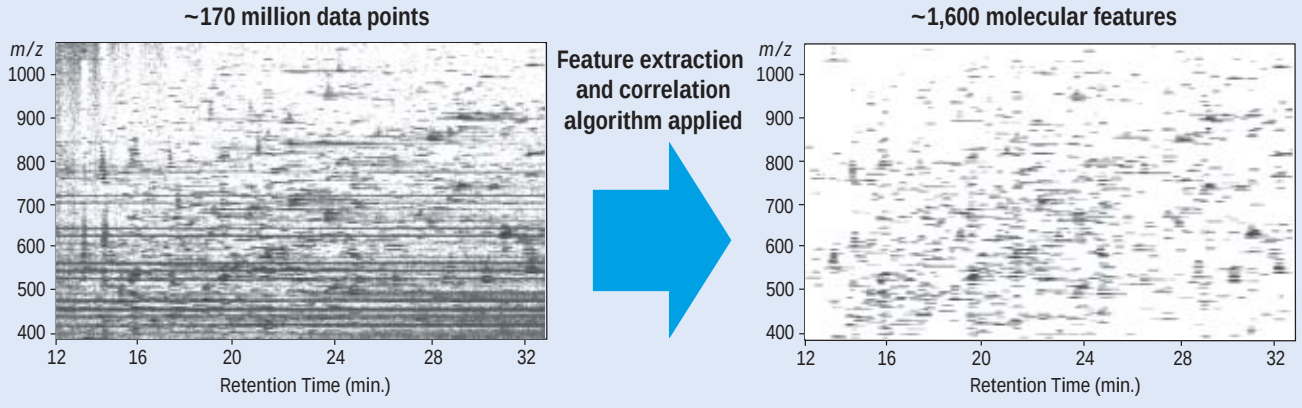
The empirical formula generation program produces a list of most likely identities based on accurate mass data and your sample knowledge and priorities

Turning raw data into useful data

A powerful new feature extraction and correlation algorithm enhances qualitative analysis of complex mixtures of peptides or smaller molecules. By identifying related information in raw data, it improves the accuracy of subsequent empirical formula determination or database searching.

The feature extraction and correlation algorithm locates the groups of co-variant ions in a chromatogram. Each of these groups represents a unique compound. Thus, the algorithm identifies all the components in a chromatogram, instead of just identifying chromatographic peaks, which may conceal multiple components. This facilitates very effective removal of chemical background data.

After identifying components and removing background, the algorithm assigns charge states. It also identifies adducts so the molecular ion and adduct ion can be treated as a single compound. Further, the algorithm identifies isotopes, and reports only monoisotopic masses for more accurate empirical formula determination and database searches.



Processing of raw data with the feature extraction and correlation algorithm identifies approximately 1600 compounds out of 170 million raw data points from a sample of BSA spiked with myoglobin. These examples zoom in on a small region of the total data display.

Turning proteomic data into answers

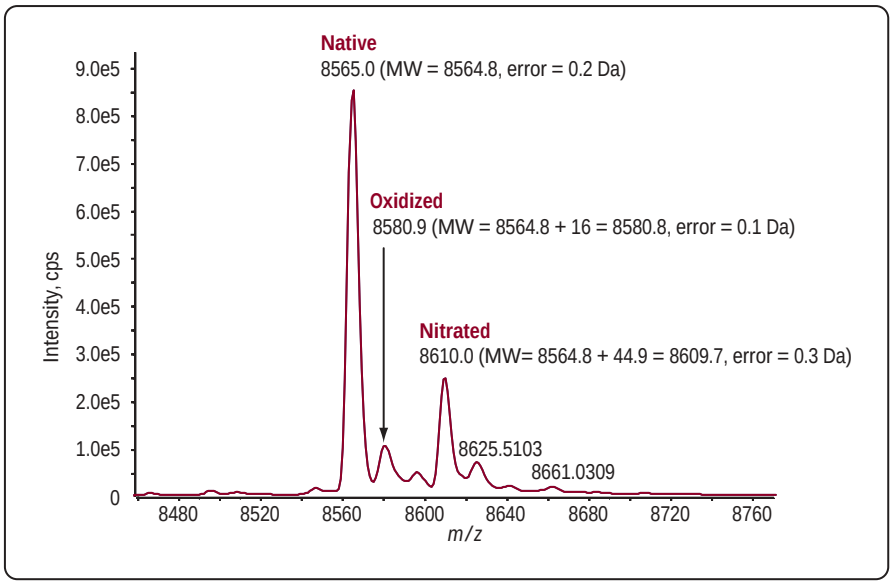
The outstanding mass accuracy, resolution, and reproducibility of the 6210 TOF make it a great platform for protein research. Refined software packages for protein confirmation and expression profiling make it easier to turn superior data into useful answers.

Confirm identities and identify variants with bioconfirmation software

If your research involves synthesis of recombinant proteins or peptides, the Agilent MassHunter Bioconfirmation software will help you confirm identities and identify variants before you start expensive testing.

More accurate results with optimized deconvolution

Analysis of both protein and peptide spectra begins with deconvolution. Unlike some competing software, the bioconfirmation software contains separate deconvolution algorithms, one optimized for proteins and the other for peptides.



The MassHunter Bioconfirmation software discerns modified forms of proteins, as shown in this deconvoluted spectrum of three major products in a peroxynitrite-treated ubiquitin sample

Sample Name: Beta-Lac-2pmol Method Name: F:\TOF\damethods\protein_small_fol_25.anm
Data File Name: F:\TOF\data\BetaLac.wiff Acq Time: March 16 2004, 09:52:16 AM

TargetProteins

Protein	Target Mass Average (Da)	Measured Mass Average (Da)	Measured Mass Apex (Da)	Area	+/- (Da)
	18277.1700	18277.1391	18277.0266	1238472.6971	-0.0309
	18363.2600	18363.2551	18363.0266	1298021.2043	-0.0049

A and B variants

OtherProteins

Measured Mass Average (Da)	Measured Mass Apex (Da)	Area	Time (min)
18363.2551	18363.0266	1298021.2043	3.76
18277.1391	18277.0266	1238472.6971	3.76
18362.9925	18376.0266	922081.2178	3.76
18410.6222	18410.0266	265030.2922	3.76
18297.0366	18297.0266	258021.0757	3.76
18461.2824	18461.0266	187922.8999	3.76
18324.1605	18324.0266	163183.0441	3.76
18396.7208	18396.0266	118587.3214	3.76

Other, non-target proteins found

A portion of the Protein Confirmation Report from analysis of β-lactoglobulin, showing target proteins (the A and B variants) confirmed with low-ppm mass errors

Better molecular feature extraction enhances peptide identification

MassHunter Bioconfirmation software uses the feature extraction and correlation algorithm to very accurately locate all of the compounds—not just all of the peaks—in complex peptide mixtures. You can import the resulting mass lists into a database search program, such as Agilent's Spectrum Mill for MassHunter software, for fast identification by peptide mass fingerprinting.

Quick, efficient confirmation for recombinant proteins...

The bioconfirmation software helps you quickly and efficiently confirm the identities of intact, recombinant proteins. For each sample, it generates a protein confirmation report that verifies the expected protein, and lists molecular weights and other data for unanticipated variants and impurities.

...and identification of unexpected variants

When identity confirmation finds unexpected variants, proteolytic digestion and reanalysis with the bioconfirmation software's peptide mass mapping function can identify the parts of the actual sequence that match the expected sequence and the parts that do not; providing valuable information about the site and nature of the variation.

Expression profiling software for efficient biomarker discovery — and more

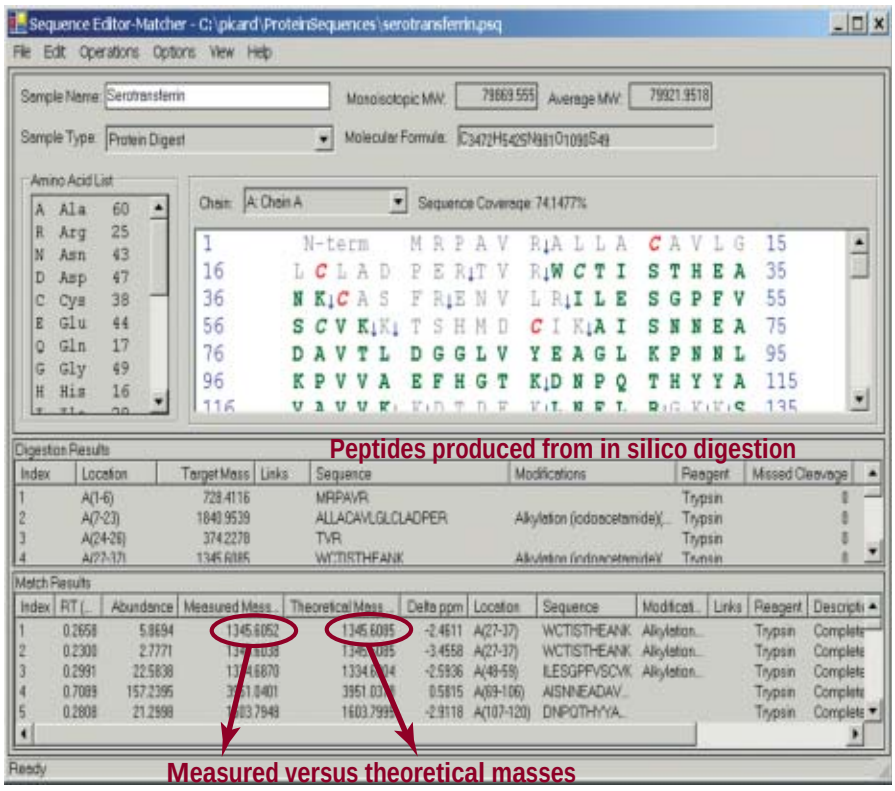
With appropriate Agilent LC and ion source choices, the 6210 TOF is an outstanding tool for fast, efficient expression profiling. Agilent's MassHunter Profiling software facilitates this with optimized tools for both compound location and data visualization. Another application is the QA/QC of glycoproteins through expression profiling of free glycans.

Superior location of compounds

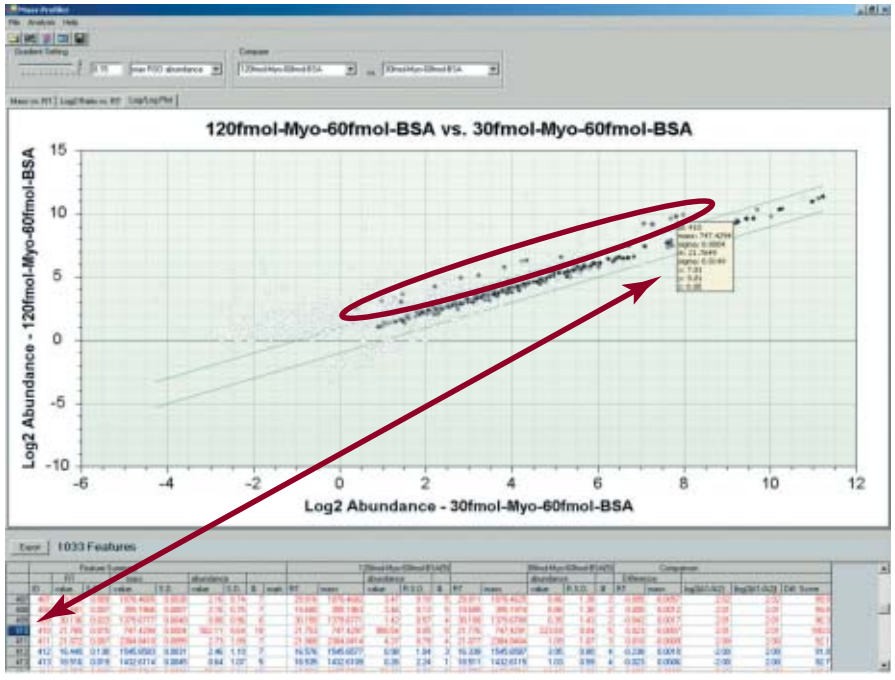
MassHunter Profiling software uses the feature extraction and correlation algorithm, which does a better job of locating all the components in even very complex peptide mixtures.

Powerful statistical comparison and visualization

The MassHunter Profiling software statistically compares results from two samples and displays multiple variables such as mass, retention time, and abundance, in tables or graphs.



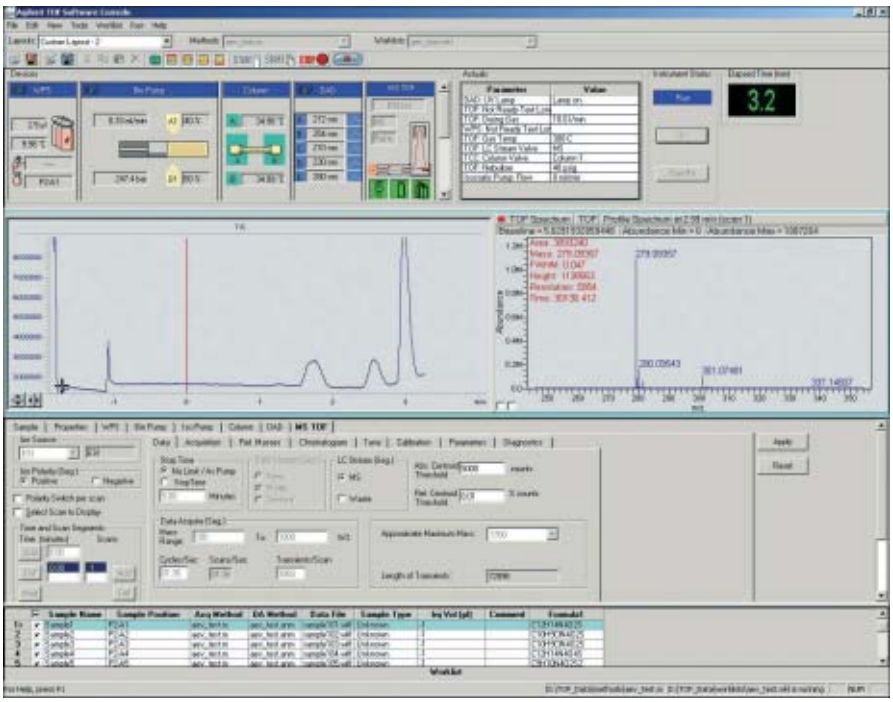
When analysis of recombinant proteins indicates that the wrong protein was produced, the interactive sequence editor/matcher helps locate the site of the variation



BSA spiked with two different levels of myoglobin simulates a biological sample with differentially expressed proteins. The MassHunter Profiling software clearly identifies myoglobin ions present at different "expression levels." Specific information about each feature is displayed in the feature table and can be displayed in individual pop-up boxes.

Maximum productivity from well-designed software

The 6210 TOF uses Agilent's MassHunter Workstation data acquisition software to simplify setup and operation, and to maximize throughput—regardless of application. Additional productivity-enhancing software facilitates shared, walk-up access by multiple users and remote data review.



Easy-to-use, yet full-featured instrument control and data acquisition software puts complete control at your fingertips

Faster, easier setup and acquisition

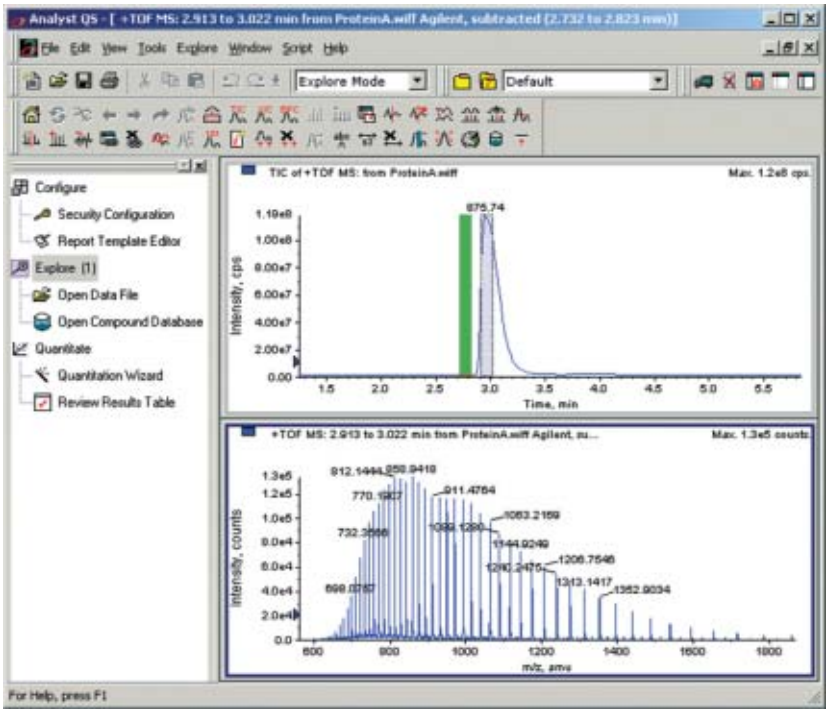
Whether you are an expert or new to LC/MS, MassHunter Workstation software greatly simplifies operation of your LC/MS system.

- Tune automatically – A proven, reliable autotune program maximizes performance and minimizes effort.
- Save time setting up analyses – Import worklists directly from spread sheet programs such as Microsoft® Excel.
- Operate from a single user interface – A single interface for both LC and MS can be configured to display only the information you need.

Powerful data analysis

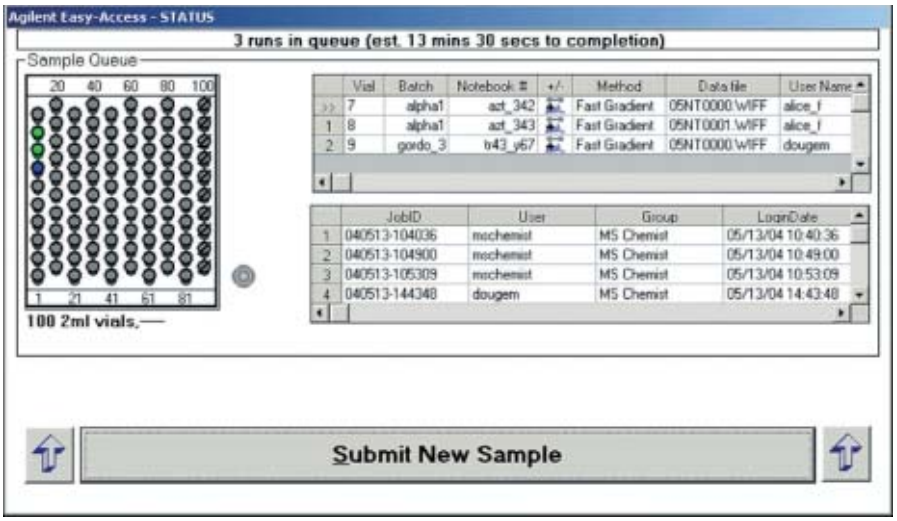
The data analysis software provides both qualitative and quantitative answers. It can be further empowered with application-specific software packages for small molecule confirmation and identification, or protein confirmation and expression profiling.

The data analysis software includes a wealth of tools for efficient qualitative and quantitative analysis



Easy, walk-up access to 2-ppm accurate mass measurements

Agilent MassHunter Easy Access software facilitates access to far better mass accuracy than has ever been available in a walk-up system before. The MassHunter Easy Access software allows you to simply ”walk up“ to your TOF, input basic sample information, and choose an analytical method from a list. The software even shows you where to place the sample vial. Results are distributed by e-mail, and can be configured to include only the information you need.



Easy access software presents a simplified user interface, making it easier for everyone, from experts to novices, to confirm synthesis products or identify unknowns

Remote review of TOF data, regardless of application, is facilitated by the data browser software.

Data Browser software facilitates remote data review

The Agilent Data Browser software enables you to review all of your TOF results without having TOF software loaded on your PC. It is an ideal complement to the walk-up capabilities of the easy access software; easy access software automatically e-mails data files to your office PC, where the data browser software provides fast, straightforward data review.

For high-throughput confirmation, the data browser software displays results for an entire well-plate in a single graphic. Convenient color coding shows, at a glance, which syntheses were successful. It can also provide mass error and sample purity information.

For analysis of unknowns, the data browser software provides empirical formulas or the results of database searches.

For more information

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Specifications

Mass Range
m/z 50–12,000

Mass Accuracy
< 2 ppm, RMS, measured at the $(M + H)^+$ ion of reserpine (*m/z* 609.2807) using internal mass reference

Resolution
Greater than 13,000 measured at *m/z* 2722

Spectral Acquisition Rate
20 spectra/second from *m/z* 100 to 3,000

40 spectra/second from *m/z* 100 to 1,000

Sensitivity Specification
> 10:1 signal-to-noise (peak-to-peak) at the $(M + H)^+$ ion at *m/z* 609.2807 for LC/MS injection of 10 pg reserpine on column

Conditions
Column – ZORBAX Rapid Resolution SB-C18 2.1–30 mm 3.5 micron

Mobile phase – 25% water
75% methanol 5 mM ammonium acetate

Flow rate – 400 µL/min

Polarity Switching
Spectrum-to-spectrum polarity switching at 1 complete positive/negative cycle/second

Global service and support

Agilent has earned its reputation for one of the finest service and support organizations in the life science and chemical analysis industries. Our sophisticated communications technology and infrastructure enable us to operate seamlessly in more than 40 countries; so we can support you wherever you are. Yet our global perspective does not stop us from being responsive down to the last local detail.

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